Title

CRYSTAL STRUCTURE OF BIS (PENTAMETHYLCYCLOPENT-ADIENYL)BIS(PYRIDINE)YTTERBIUM(II)

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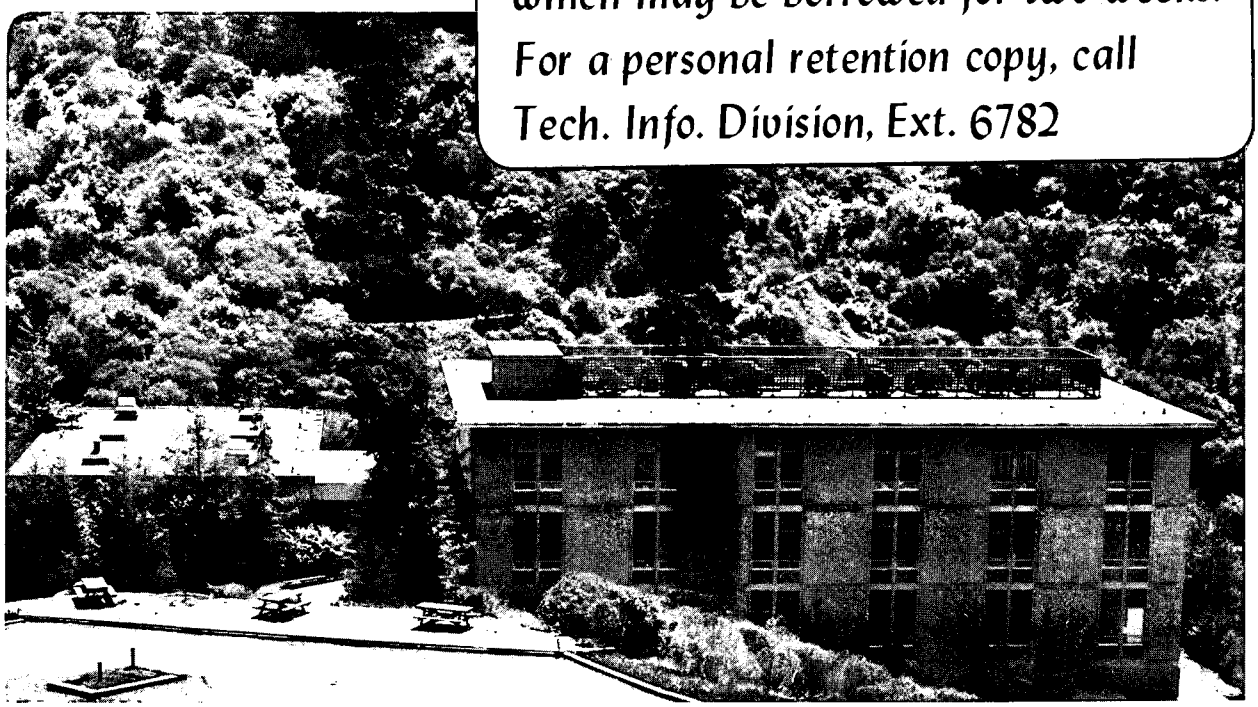

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CRYSTAL STRUCTURE OF BIS(PENTAMETHYLCYCLOPENTADIENYL)BIS(PYRIDINE)YTTERBIUM(II)

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SEPTEMBER 1981

ABSTRACT

Crystals of $(C_5Me_5)_2Yb(C_5H_5N)_2$ crystallize in the monoclinic system, $P2_1/c$, with $\underline{a}$ = 16.092(6) Å, $\underline{b}$ = 9.883(4) Å, $\underline{c}$ = 17.872(7) Å, and β = 98.46(3)° at 21°C. For Z = 4 the calculated density is 1.42 g cm^{-3}. Two pentamethyl cyclopentadienyl rings and the nitrogen atoms of the two pyridine molecules coordinate to the Yb atom in a distorted tetrahedral arrangement with approximate C_2 symmetry. The Yb-N distances average 2.56 Å, the Yb-C distances average 2.74 Å, and the Yb-Cp (centers) average 2.46 Å. The C_5Me_5 rings are in a staggered configuration with respect to each other. The methyl groups of the C_5Me_5 rings are bent 0.13 to 0.31 Å out of the planes of the C_5 rings away from the Yb atom. The 3278 data with $F^2 > 3\sigma$ refined by full matrix least squares to an R factor of 0.031.

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INTRODUCTION

Bonding of cyclopentadienyl groups and its substituted analogues to f-block metals is thought to be predominantly ionic, i.e., there is very little electron exchange between the metal atom and the organic ligand. A structural criterion has been advanced by Raymond that is remarkably accurate in predicting f-metal to carbon bond lengths, given the simplicity and therefore utility of the model.[1] The fundamental principle of the model is that metal-carbon bond lengths are a sensitive function of the oxidation state and coordination number of a given metal ion. Subtraction of the ionic radius of a metal atom, which is a function of the oxidation state and coordination number, from the observed metal-carbon bond length gives the effective ionic radius of a cyclopentadienyl group. Though ligand-ligand repulsions also play a role in determining the metal-carbon bond length, for the f-block metals the effective ionic radius of the cyclopentadienyl ligand is observed to be fairly constant, 1.64 ± 0.04 Å. Thus, it may be said that the bonding in these organometallic molecules is largely ionic.

In the course of our investigations into the chemistry of pentamethylcyclopentadienyl derivatives of the lanthanide metals, we have prepared a number of compounds whose structures can be used to test this model. The compound whose structure is reported here, $(C_5Me_5)_2Yb(py)_2$, offers an interesting test of the ionic bonding model for divalent lanthanide complexes, since its coordination number is one greater than that of the divalent $(C_5Me_5)_2Yb(thf)$, which has been structurally characterized.[2]

RESULTS AND DISCUSSION

The compound $Yb(C_5Me_5)_2(py)_2$ is prepared by the reaction of $Yb(C_5Me_5)_2(OEt_2)$ and excess pyridine in toluene, and crystallizes from toluene as dark green prisms.

An ORTEP view of the molecule (Fig. 1) shows a distorted tetrahedral array of the ligands about ytterbium, with approximate C_2 symmetry. Atomic positions and selected distances and angles are given in Tables I-III. The angles about the coordination sphere range from 136.3(3)° for the C_5Me_5 centroid-Yb-C_5Me_5 centroid angle to 82.5(2)° for the N(1)-Yb-N(2) angle. The pyridine rings have normal geometry, as do the C_5Me_5 rings, which are arranged in a staggered conformation (Fig. 2).

The displacements of the methyl carbon atoms from the planes of their respective C_5 rings, which range from 0.13 to 0.31 Å, are greater than the corresponding displacements in $Yb(C_5Me_5)_2(thf)$, which range from 0.03 to 0.21 Å. This is a result of more steric crowding in $Yb(C_5Me_5)_2(py)_2$, which has a higher coordination number.

The pyridine rings are directed almost linearly away from the ytterbium atom (< Yb-N(1)-C(23) = 171.0(4)° and < Yb-N(2)-C(28) = 174.6(3)°), and the planes of the pyridine rings are canted by ca. 35° from the plane of Yb, N(1) and N(2). The Yb-N(1) and Yb-N(2) distances are 2.586(7) and 2.544(6) Å, respectively. If one subtracts the ionic radius of a eight-coordinate ytterbium(II) ion, 1.14 Å,[3] from the Yb-N distances, one obtains 1.45 and 1.40 Å, respectively, for the ionic radii of the pyridine nitrogen atoms. A value of 1.40 Å can be calculated from the

structure of the eight-coordinate bis(pyridine)tris(2,2,6,6-tetramethylheptane-3,5-dionato)europium(III).[4]

Though the ytterbium-carbon distances in ring 1 do not show any systematic variation, those in the ring 2 range from 2.691(8) Å for C(14) to 2.786(9) Å for C(11), resulting in a tilt by ring 2 of ca. 2° away from the nitrogen atoms. The average ytterbium-carbon distance is 2.74(4) Å, which is 0.08 Å greater than the corresponding average in $Yb(C_5Me_5)_2(thf)$ [2.66(2) Å]. Thus, if one counts the C_5Me_5 ligand as being three-coordinate, the ionic radius of ytterbium(II) in eight-coordination is 0.08 Å greater than that in seven-coordination. Shannon suggests a difference of 0.06 Å.

Using the ionic radii tabulated by Shannon,[3] one can estimate the effective ionic radius of the C_5Me_5 ligand in the bis(pentamethylcyclopentadienyl)ytterbium complexes that have been structurally characterized. As shown in Table IV, these radii are consistent with the value suggested by Raymond for predominantly ionic bonding, 1.64 ± 0.03 Å. Based on these structural data alone, the bonding in ytterbium(II) pentamethylcyclopentadienyl complexes appears to be largely ionic, and in this regard does not differ greatly from the bonding observed in ytterbium(III) cyclopentadienyl complexes.

EXPERIMENTAL SECTION

Bis(pentamethylcyclopentadienyl)bis(pyridine)ytterbium(II). Pyridine (1 mL, an excess) was added to (diethyl ether) bis(pentamethylcyclopentadienyl)ytterbium(II) (1.75 g, 3.38 mmol) dissolved in toluene (15 mL). A dark green solid precipitated. After stirring the mixture for 1 h, the volatile material was removed under reduced pressure. The residue was washed with pentane (2 x 30 mL) and extracted into toluene by stirring overnight (2 x 100 mL). The combined extracts were concentrated to ca. 60 mL and cooling (-10°C), resulted in formation of green prisms, yield 1.77 g (87%). When heated in a sealed capillary, the compound darkens above ca. 190°C and melts 208-210°C. ^{1}H NMR (26°C, d_6-benzene): ∂ 2.12 (s, C_5Me_5). Resonances due to coordinated pyridine were not observed. Anal. Calcd. for $C_{30}H_{40}N_2Yb$: C, 59.9; H, 6.70; N, 4.66. Found: C, 60.3; H, 6.70; N, 4.47. IR (Nujol): 3092w, 3063w, 3037w, 2720w, 1594s, 1486w, 1213m, 1159m, 1107w, 1069m, 1033m, 998m, 984w, 942w, 886w, 800w, 759s, 729w, 702s, 662m, 618m, 591m, and 419m cm^{-1}.

X-Ray. Crystals of the complex were sealed in quartz capillaries under an atmosphere of argon. Preliminary Weissenberg photography showed the crystal to be monoclinic. A crystal of dimensions 0.06 x 0.22 x 0.22 mm was examined with a Picker FACS-I automated diffractometer equipped with a graphite monochromator and a Mo X-ray tube. ω-scans of several low-angle peaks had a width at half-height of 0.15°. Least-squares refinement of the setting angles of 12 manually centered reflections (45° < 2θ < 50°) using Mo Kα_1 (λ =

0.70930 Å) radiation gave $\underline{a}$ = 16.092(6) Å, $\underline{b}$ = 9.883(4) Å, $\underline{c}$ = 17.872(7) Å, β = 98.46(3)°, and V = 2811.4 $Å^3$ at 21(1)°C. The observed extinctions are unique to space group $P2_1/c$. For Z = 4 and a molecular weight of 601.70 g mol^{-1} the calculated density is 1.42 g cm^{-3}.

Intensity data for two forms (±h+k±l) to 50° in 2θ were collected using θ-2θ scans with a scan speed of 2°/min on 2θ, a scan range from 0.9° below the $K\alpha_1$ peak to 0.9° above the $K\alpha_2$ peak, and with backgrounds counted for 4 seconds at each end of the scan range. Three standard reflections, measured after every 150 reflections decreased in intensity by 2% during data collection and the measured intensities were corrected accordingly. Early intensity measurements affected by slow movement in the capillary were deleted and those reflections remeasured. Thereafter, the orientation matrix was recalculated twice daily, which proved sufficient to compensate for crystal movement.

An analytical absorption correction was applied[5] (μ = 33.3 cm^{-1} for MoKα) with the crystal described by the [100], [010], and [001] faces and the crystal dimensions adjusted to fit the intensity variation of 11 azimuthal scans. Maximum and minimum correction factors were 2.42 and 1.27, respectively. Intensities of the 10,699 reflections measured were corrected for absorption, Lorentz and polarization factors,[6] extinctions were removed, and equivalent reflection were averaged to obtain a set of 4985 unique reflections.

Trial coordinates for the ytterbium atom were obtained from a three-dimensional Patterson function and were refined by least-squares.

An electron density map then revealed all non-hydrogen atoms. A series of isotropic and anisotropic least-squares refinements, followed by a difference Fourier calculation, gave a map that showed pyridine hydrogen atoms but not those of the methyl groups. In the final cycles of least-squares refinement all non-hydrogen atoms were refined anisotropically with the pyridine hydrogen atoms included in their calculated positions (assuming a C-H bond distance of 0.95 Å) with a fixed isotropic thermal parameter of 8.0 $Å^2$. An empirical extinction correction was applied where $F_{corr} = (1 + 4.54 \times 10^{-8} I) F_{obs}$ where F_{corr} and F_{obs} are the corrected and observed structure factors and I is the observed intensity. The refinement converged smoothly to the positions given in Table I with the changes in parameters in the last cycle all less than 0.02 σ. Thermal parameters, hydrogen atoms positions, and structure factor amplitudes are included in the supplementary material.

The full-matrix least-squares program minimizes the function $\Sigma w|\Delta F|^2/\Sigma w F_o^2$ where the assigned weights, $w = [\sigma(F)]^{-2}$, are derived from $\sigma(F^2) = [S^2 + (pF^2)^2]^{1/2}$ where S^2 is the variance due to counting statistics and p = 0.04. Scattering factors for neutral atoms were those of Doyle and Turner[7] for Yb, N, and C with anomolous dispersion corrections[4] applied; hydrogen scattering factors of Stewart, Davidson, and Simpson[8] were used. Discrepancy indices for 298 parameters varied with 3278 data having $F^2 > 3\sigma(F^2)$ are

$$R = \Sigma||F_o|-|F_c||/\Sigma|F_o| = 0.031$$

$$R_w = \Sigma[w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2} = 0.037$$

R for all 4985 data is 0.061 and the estimated standard deviation of an observation of unit weight is 1.15. A difference Fourier calculation after the final cycle of least-squares refinement had a maximum electron density of 0.88 e $Å^{-3}$.

ACKNOWLEDGMENT

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under contract number W-7405-Eng-48. One of us (B.S.) is on leave from the Chemistry Department, Beloit College, Beloit, Wisconsin. We thank Dr. P. L. Watson for providing us with some of her X-ray structural results in advance of publication.

SUPPLEMENTARY MATERIAL AVAILABLE

Listings of anisotropic thermal parameters, calculated hydrogen positions and observed and calculated structure factors (21 pages). Ordering information is given on any current masthead.

REFERENCES

1. Raymond, K.N.; Eigenbrot, C.W. Acc. Chem. Res. 1980, 13, 276.

2. Tilley, T.D.; Andersen, R.A.; Spencer, B.; Ruben, H.; Zalkin, A.; Templeton, D.H. Inorg. Chem. 1980, 19, 2999.

3. Shannon, R.D. Acta Cryst. 1976, A32, 751.

4. Cramer, R.E.; Seff, K.; Acta Cryst. 1972, B28, 3281.

5. Templeton, L.K.; Templeton, D.H. Abstracts, American Crystallographic Proceedings, Series 2, Vol. 1, 1973, p.143.

6. Stewart, R.F.; Davidson, E.R.; Simpson, W.T. J. Chem. Phys. 1965, 42, 3175.

7. Doyle, P.A.; Turner, P.S. Acta Cryst. 1968, A24, 390.

8. Cromer, D.T.; Liberman, D. J. Chem. Phys. 1970, 53, 1891.

Table I. Positional Parameters in $(C_5Me_5)_2Yb(C_5H_5N)_2$.[a]

ATOM	X	Y	Z
YB	.24809(2)	.07142(3)	.29227(2)
N(1)	.3320(5)	.2724(7)	.3581(4)
N(2)	.1425(4)	.1403(6)	.3781(3)
C(1)	.1985(5)	.0471(6)	.1378(4)
C(2)	.1294(4)	.1069(7)	.1661(4)
C(3)	.1531(5)	.2384(7)	.1911(4)
C(4)	.2377(5)	.2589(7)	.1788(4)
C(5)	.2650(4)	.1408(7)	.1466(4)
C(6)	.1933(6)	-.0828(8)	.0899(5)
C(7)	.0408(5)	.0469(8)	.1558(4)
C(8)	.0941(6)	.3447(8)	.2152(5)
C(9)	.2841(6)	.3926(8)	.1843(5)
C(10)	.3495(5)	.1255(9)	.1183(5)
C(11)	.3247(6)	-.0951(8)	.4068(5)
C(12)	.3714(5)	-.1114(8)	.3470(5)
C(13)	.3186(5)	-.1785(7)	.2877(5)
C(14)	.2399(5)	-.1983(7)	.3111(5)
C(15)	.2436(6)	-.1476(8)	.3852(5)
C(16)	.3614(8)	-.039(1)	.4848(6)
C(17)	.4666(6)	-.085(1)	.3473(7)
C(18)	.3500(6)	-.2374(8)	.2180(6)
C(19)	.1665(6)	-.2773(9)	.2692(6)
C(20)	.1751(7)	-.165(1)	.4338(6)
C(21)	.4146(7)	.271(1)	.3705(7)
C(22)	.4634(8)	.380(1)	.3960(9)
C(23)	.4239(9)	.503(1)	.4061(7)
C(24)	.3394(7)	.5075(9)	.3939(6)
C(25)	.2963(6)	.3905(9)	.3702(5)
C(26)	.1686(5)	.1870(9)	.4474(5)
C(27)	.1152(7)	.215(1)	.4990(5)
C(28)	.0321(6)	.1929(9)	.4783(5)
C(29)	.0035(5)	.1436(9)	.4086(5)
C(30)	.0597(6)	.1194(8)	.3610(5)

[a]In this and the following tables, the number in parentheses are the the estimated standard deviations in the least significant digits.

Table II. Selected Interatomic Distances (Å).

Yb-C(1)	2.769(7)	Yb-C(11)	2.770(8)
-C(2)	2.754(7)	-C(12)	2.754(7)
-C(3)	2.742(7)	-C(13)	2.724(7)
-C(4)	2.734(6)	-C(14)	2.692(7)
-C(5)	2.743(7)	-C(15)	2.736(7)
C(1)-C(2)	1.417(9)	C(11)-C(12)	1.404(12)
C(2)-C(3)	1.409(9)	C(12)-C(13)	1.421(11)
C(3)-C(4)	1.425(9)	C(13)-C(14)	1.405(10)
C(4)-C(5)	1.400(9)	C(14)-C(15)	1.408(11)
C(5)-C(1)	1.405(9)	C(15)-C(11)	1.404(12)
C(1)-C(6)	1.539(9)	C(11)-C(16)	1.535(13)
C(2)-C(7)	1.529(10)	C(12)-C(17)	1.553(12)
C(3)-C(8)	1.520(10)	C(13)-C(18)	1.527(11)
C(4)-C(9)	1.513(10)	C(14)-C(19)	1.519(12)
C(5)-C(10)	1.527(10)	C(15)-C(20)	1.511(12)
Yb -N(1)	2.586(7)	Yb -N(2)	2.544(6)
N(1) -C(21)	1.315(12)	N(2) -C(26)	1.330(9)
N(1) -C(25)	1.333(11)	N(2) -C(30)	1.339(10)
C(21)-C(22)	1.374(14)	C(26)-C(27)	1.378(12)
C(22)-C(23)	1.394(16)	C(27)-C(28)	1.351(13)
C(23)-C(24)	1.346(15)	C(28)-C(29)	1.353(12)
C(24)-C(25)	1.383(12)	C(29)-C(30)	1.350(11)

Table III. Selected Angles (deg).

N(1)-Yb-N(2)	82.5(2)
N(1)-Yb-Cp(1)[a]	103.6(2)
N(1)-Yb-Cp(2)	111.5(3)
N(2)-Yb-Cp(1)	107.7(3)
N(2)-Yb-Cp(2)	102.0(3)
Cp(1)-Yb-Cp(2)	136.3(3)

C(5)-C(1)-C(2)	108.1(6)	C(15)-C(11)-C(12)	109.2(8)
C(1)-C(2)-C(3)	107.8(6)	C(11)-C(12)-C(13)	107.0(8)
C(2)-C(3)-C(4)	107.6(6)	C(12)-C(13)-C(14)	108.0(7)
C(3)-C(4)-C(5)	108.0(6)	C(13)-C(14)-C(15)	108.3(8)
C(4)-C(5)-C(1)	108.4(6)	C(14)-C(15)-C(11)	107.4(8)
C(2)-C(1)-C(6)	124.4(7)	C(12)-C(11)-C(16)	123.7(10)
C(5)-C(1)-C(6)	126.2(7)	C(15)-C(11)-C(16)	126.9(10)
C(1)-C(2)-C(7)	124.2(6)	C(11)-C(12)-C(17)	128.0(9)
C(3)-C(2)-C(7)	126.9(7)	C(13)-C(12)-C(17)	124.3(9)
C(2)-C(3)-C(8)	125.1(7)	C(12)-C(13)-C(18)	123.6(8)
C(4)-C(3)-C(8)	126.6(6)	C(14)-C(13)-C(18)	127.7(8)
C(3)-C(4)-C(9)	126.0(7)	C(13)-C(14)-C(19)	126.5(8)
C(5)-C(4)-C(9)	125.0(7)	C(15)-C(14)-C(19)	124.7(8)
C(4)-C(5)-C(10)	124.5(7)	C(14)-C(15)-C(20)	124.5(9)
C(1)-C(5)-C(10)	126.7(7)	C(11)-C(15)-C(20)	127.7(9)
C(21)-N(1)-C(25)	115.7(8)	C(26)-N(2) -C(30)	115.8(7)
N(1)-C(21)-C(22)	124.1(10)	N(2) -C(26)-C(27)	123.3(8)
N(1)-C(25)-C(24)	125.0(9)	N(2) -C(30)-C(29)	124.3(8)
C(21)-C(22)-C(23)	118.6(11)	C(26)-C(27)-C(28)	118.4(8)
C(22)-C(23)-C(24)	118.6(10)	C(27)-C(28)-C(29)	119.8(8)
C(23)-C(24)-C(25)	118.0(10)	C(28)-C(29)-C(30)	118.4(8)

[a]Cp is the centroid of a C_5Me_5 ring.

Table IV. Effective Ionic Radius (Å) of the Me_5C_5 Group.

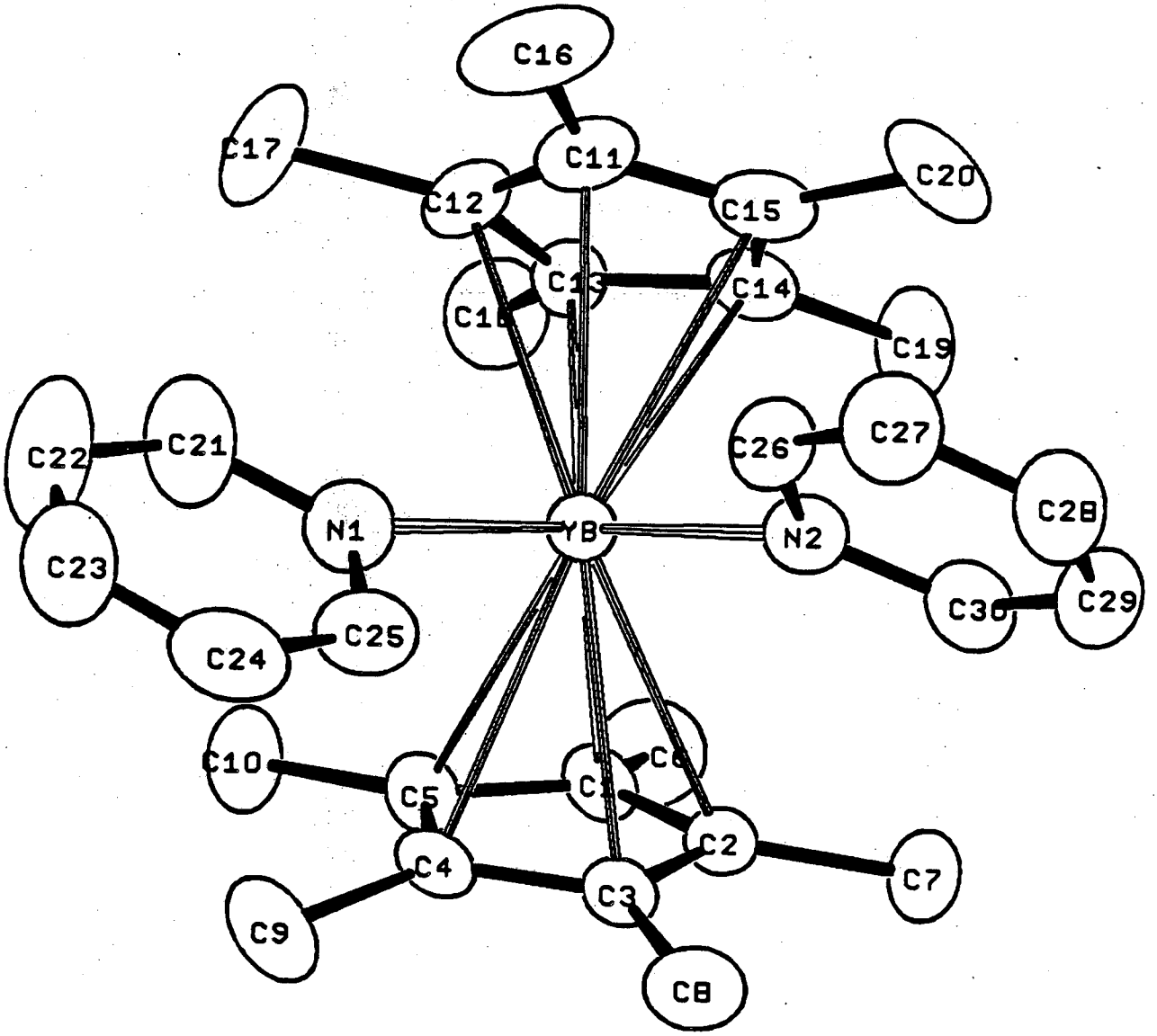
Compound	M-C bond length, Å	metal ion radius, Å	effective $C_5Me_5^-$ radius, Å	Reference
$Yb(C_5Me_5)_2(py)_2$	2.74(4)	1.14	1.60	this work
$Yb(C_5Me_5)_2(thf)$	2.66(2)	1.08	1.58	a
$Yb(C_5Me_5)_2(S_2CNEt_2)$	2.63(3)	0.985	1.64	b
$Yb(C_5Me_5)_2(thf)[Co(CO)_4]$	2.596(2)	0.985	1.61	c
$[Yb(C_5Me_5)_2]_2[Fe_3(CO)_{11}]$	2.57(1)	0.985	1.59	d
$[Li(OEt_2)_2][(C_5Me_5)_2YbCl_2]$	2.611(4)	0.985	1.63	e
$Yb(C_5Me_5)_2AlCl_4$	2.584(5)	0.985	1.60	e

a. Reference 2.
b. T.D. Tilley, R.A. Andersen, A. Zalkin, and D.H. Templeton, submitted.
c. T.D. Tilley and R.A. Andersen, J. Chem. Soc. Chem. Comm. in press.
d. T.D. Tilley and R.A. Andersen, submitted.
e. P.L. Watson, J.F. Whitney, and R.L. Harlow, Inorg. Chem. in press.

FIGURE CAPTIONS

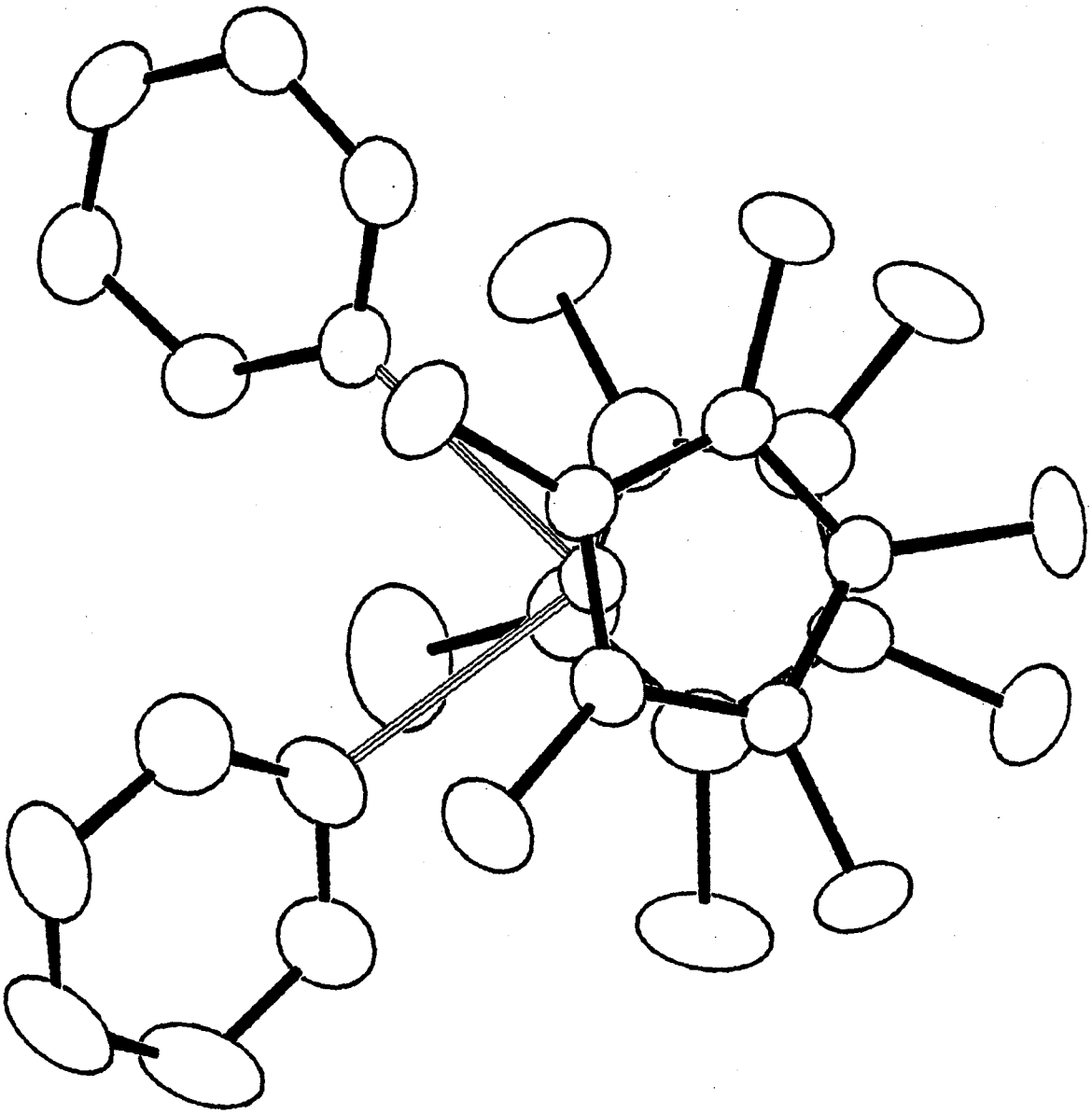
Fig. 1. ORTEP drawing of $(C_5Me_5)_2Yb(C_5H_5N)_2$ as viewed down the pseudo 2-fold axis.

Fig. 2. ORTEP drawing looking down the centers of the pentamethylcyclopentadiene rings showing the staggered configurations of the rings with respect to each other.



XBL 798-10946

Fig. 1



XBL 799-11776

Fig. 2

SUPPLEMENTARY MATERIAL

CRYSTAL STRUCTURE OF BIS(PENTAMETHYLCYCLOPENTADIENYL)BIS(PYRIDINE)YTTERBIUM(II)

T. Don Tilley, Richard A. Andersen, Brock Spencer, and Allan Zalkin*

1. Anisotropic thermal parameters for $(C_5Me_5)_2Yb(C_4H_5N)_2$.
2. Calculated atomic positional parameters for the toluene hydrogen atoms.
3. Observed structure factors (19 pages).

Anisotropic Thermal Parameters for $(C_5Me_5)Yb(C_4H_5N)_2$.[a]

ATOM	B11	B22	B33	B12	B13	B23
YB	3.01(1)	2.58(1)	2.93(1)	-.06(1)	.407(8)	-.06(2)
N(1)	5.4(4)	4.5(3)	5.2(4)	-1.2(3)	.4(3)	-.2(3)
N(2)	4.4(3)	4.2(3)	3.1(3)	.4(2)	.9(2)	.0(2)
C(1)	4.3(4)	3.1(3)	2.9(3)	-.3(3)	.9(3)	-.4(2)
C(2)	3.4(3)	3.7(3)	2.7(3)	-.1(2)	.6(2)	.3(2)
C(3)	4.3(4)	3.0(3)	2.9(3)	.5(3)	.8(3)	.4(2)
C(4)	4.3(4)	3.0(3)	3.1(3)	-.4(3)	.7(3)	.7(2)
C(5)	3.3(3)	3.5(3)	3.5(3)	-.2(3)	1.2(3)	-.1(3)
C(6)	7.8(6)	4.8(4)	4.5(4)	-.1(4)	.9(4)	-2.3(4)
C(7)	3.6(3)	5.9(5)	4.5(4)	-1.7(3)	.1(3)	.0(3)
C(8)	5.9(5)	4.0(4)	6.0(5)	2.2(3)	1.7(4)	.6(3)
C(9)	7.3(5)	3.9(4)	6.3(5)	-2.0(3)	2.1(4)	.2(3)
C(10)	4.5(4)	6.0(4)	6.7(5)	.1(4)	2.4(4)	.4(4)
C(11)	5.7(5)	5.1(4)	4.5(4)	1.9(4)	-.3(4)	.9(3)
C(12)	3.2(4)	4.3(4)	7.1(5)	1.3(3)	.0(4)	.8(3)
C(13)	4.3(4)	3.1(3)	5.0(4)	.5(3)	1.1(3)	.3(3)
C(14)	4.4(4)	2.9(3)	6.4(5)	1.0(3)	1.4(4)	1.4(3)
C(15)	5.4(5)	4.1(4)	5.5(5)	1.5(3)	1.6(4)	2.0(4)
C(16)	11.3(9)	9.3(8)	5.5(5)	2.8(6)	-3.0(5)	-.5(5)
C(17)	3.5(4)	7.4(6)	12.3(9)	.8(4)	-.2(5)	-.2(6)
C(18)	6.7(5)	4.3(4)	8.7(6)	1.4(4)	3.2(5)	-1.0(4)
C(19)	5.2(5)	4.2(4)	10.6(7)	-1.5(4)	.6(5)	-.5(4)
C(20)	9.5(7)	6.2(5)	8.1(6)	1.2(5)	5.4(6)	3.1(5)
C(21)	6.1(6)	5.9(5)	9.9(7)	-1.7(5)	2.9(5)	-1.9(5)
C(22)	5.8(6)	8.6(7)	15.1(11)	-2.6(6)	2.2(7)	-2.6(7)
C(23)	8.6(8)	6.5(6)	7.9(7)	-3.1(6)	.4(6)	-1.8(5)
C(24)	8.0(7)	3.9(4)	5.8(5)	-.4(4)	.1(5)	-.1(4)
C(25)	5.8(5)	5.2(5)	5.5(5)	.3(4)	.4(4)	.4(4)
C(26)	4.6(4)	6.5(5)	3.6(4)	-.4(4)	.3(3)	-.4(4)
C(27)	7.1(6)	7.7(6)	3.9(4)	-.7(5)	1.2(4)	-1.5(4)
C(28)	5.7(5)	7.0(5)	5.2(5)	-.2(4)	2.8(4)	-1.4(4)
C(29)	4.2(4)	5.6(4)	5.6(5)	-.5(3)	1.0(4)	-.5(4)
C(30)	5.7(5)	4.2(3)	4.1(4)	-.3(3)	.6(4)	-.5(3)

[a]The anisotropic temperature factor has the form $\exp(-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \ldots))$.

Calculated Atomic Parameters for the Toluene Hydrogen Atoms in $(C_5Me_5)_2Yb(C_4H_5N)_2$.

Atom	x	y	z	B, Å^2[a]
H(1)	.4432	.1881	.3611	8.000
H(2)	.5244	.3704	.4027	8.000
H(3)	.4593	.5764	.424	8.000
H(4)	.3125	.5885	.4030	8.000
H(5)	.2362	.3946	.3602	8.000
H(6)	.2274	.1983	.462	8.000
H(7)	.1384	.2486	.5473	8.000
H(8)	-.0064	.2104	.5128	8.000
H(9)	-.0547	.1263	.3916	8.000
H(10)	.0402	.0856	.3119	8.000

[a]The form of the isotropic thermal parameter is exp-B($\sin^2\theta/\lambda^2$).

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
YB.(C5(CH3)5)2.(CH5N)2 F(0,0,0) = 3279

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		0,	0	19	52	20	8*	8	313	7	-7	2	236	5	-6	-16	248	6	4
2	890	18	84	20	49	57	-14*	9	177	5	-3	3	158	5	-3	-14	237	6	5
4	231	7	-12	H,K=		0,	3	10	149	5	-5	4	219	6	-4	-12	13	31	8*
6	185	6	19	1	257	6	4	11	62	9	1	5	102	6	-2	-10	370	8	4
8	172	4	-1	2	157	4	-25	12	39	40	17*	6	0	42	-2*	-8	495	10	-0
10	522	11	19	3	31	21	-6*	13	52	20	3*	7	40	23	-15*	-6	501	10	19
12	447	10	7	4	487	10	-30	14	108	10	-0	8	163	7	1	-4	536	11	-34
14	321	7	0	5	163	4	2	15	98	7	-6	9	96	6	2	-2	569	12	-61
16	131	9	9	6	649	13	7	16	160	7	4	10	189	5	-2	2	611	12	-73
18	43	47	20*	7	37	10	-6*	17	137	13	3	11	95	7	-5	4	178	5	-16
20	106	9	1	8	564	12	8	18	145	6	-5	12	190	6	-2	6	638	13	1
H,K=		0,	1	9	32	27	6*	19	80	11	-5	13	87	7	3	8	599	12	11
1	236	5	23	10	174	4	4	H,K=		0,	6	14	159	9	-2	10	334	7	4
2	34	3	-43	11	47	11	15*	0	493	11	9	15	49	18	6*	12	39	25	19*
3	337	7	-8	12	79	7	12	1	194	4	-2	H,K=		0,	9	14	199	6	2
4	92	5	18	13	0	34	-7*	2	432	9	-7	1	76	7	2	16	257	6	4
5	879	18	48	14	207	5	-0	3	139	4	-3	2	116	5	-10	18	220	6	7
6	102	5	3	15	13	36	-26*	4	176	4	6	3	149	5	3	20	171	6	12
7	583	17	-9	16	212	7	-7	5	78	10	-4	4	188	5	1	H,K=		1,	1
8	187	5	-2	17	56	14	-1*	6	72	7	-2	5	148	5	-10	-21	105	11	-0
9	366	8	22	18	177	6	1	7	47	11	-4*	6	205	5	-1	-20	23	42	-20*
10	216	5	7	19	30	39	1*	8	189	5	-4	7	173	6	-1	-19	65	12	5
11	73	8	-4	20	114	10	6	9	111	9	-2	8	145	6	3	-18	32	36	20*
12	35	27	6*	H,K=		0,	4	10	249	6	-4	9	114	7	-9	-17	38	26	-10*
13	122	6	-6	0	300	6	17	11	127	7	-5	10	78	12	1	-16	21	57	12*
14	82	17	-7*	1	668	14	-0	12	222	5	-1	11	46	38	14*	-15	199	7	6
15	227	7	2	2	101	3	1	13	86	8	-13	12	14	34	5*	-14	146	5	10
16	121	6	-2	3	508	10	7	14	173	5	0	13	48	15	5*	-13	311	7	13
17	211	6	7	4	165	4	8	15	62	10	11	H,K=		0,	10	-12	183	5	9
18	97	8	1	5	47	7	-0	16	83	9	6	0	53	17	-6*	-11	407	9	13
19	164	6	1	6	0	25	-31*	17	56	12	31*	1	199	6	-8	-10	136	5	-4
20	54	17	-5*	7	152	4	-1	18	42	24	18*	2	42	16	-16*	-9	415	16	3
H,K=		0,	2	8	19	27	10*	H,K=		0,	7	3	165	5	-2	-8	56	7	-2
0	192	8	12	9	327	7	-2	1	104	7	5	4	31	41	10*	-7	260	6	7
1	414	9	-31	10	38	28	-19*	2	37	16	8*	5	44	19	-8*	-6	195	6	-10
2	208	5	-28	11	363	8	2	3	244	5	2	6	39	17	33*	-5	254	7	7
3	351	8	10	12	94	7	1	4	32	28	23*	7	86	7	17	-4	105	4	1
4	25	38	6*	13	340	8	-2	5	387	8	-3	8	28	32	12*	-3	308	7	-37
5	44	20	-16*	14	48	35	-12*	6	46	12	3*	9	133	5	6	-2	245	5	9
6	52	11	-15*	15	182	5	7	7	327	7	-1	10	0	35	-25*	-1	808	16	51
7	142	4	6	16	38	22	-4*	8	45	20	15*	11	164	5	5	0	533	12	-42
8	127	4	-4	17	30	42	-14*	9	198	7	2	H,K=		0,	11	1	972	22	-36
9	170	4	-5	18	19	42	8*	10	53	12	-17*	1	31	32	11*	2	260	5	10
10	255	6	5	19	38	31	-12*	11	32	27	8*	2	95	7	-3	3	210	7	-58
11	299	8	-2	H,K=		0,	5	12	37	39	-0*	3	50	21	-5*	4	200	7	31
12	203	5	2	1	66	5	3	13	79	9	7	4	165	7	1	5	91	13	11
13	283	6	-4	2	184	4	-3	14	14	38	7*	5	58	11	-5*	6	288	6	23
14	164	6	0	3	322	7	-15	15	133	6	-4	6	173	6	-3	7	100	6	2
15	141	7	-5	4	362	8	-4	16	36	30	8*	7	55	11	21*	8	109	5	-0
16	111	8	-3	5	229	5	-6	H,K=		0,	8	H,K=		1,	0	9	201	5	4
17	31	68	-5*	6	402	9	-0	0	235	6	-5	-20	167	8	2	10	100	6	-6
18	22	51	7*	7	263	6	4	1	102	7	-0	-18	228	6	3	11	370	8	1

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
12	222	6	0	-16	87	8	-5	-1	187	5	17	15	135	7	-1	-3	336	7	-3
13	366	8	3	-15	85	13	-4	0	67	5	-3	16	68	11	16	-2	47	14	20*
14	119	14	2	-14	266	8	-0	1	84	8	-7	17	53	17	8*	-1	424	9	-5
15	229	7	5	-13	49	13	-8*	2	93	6	-7	18	36	42	21*	0	69	10	-3
16	16	38	-3*	-12	416	9	-4	3	477	10	6	H,K=		1,	6	1	348	7	2
17	23	39	-12*	-11	24	31	-10*	4	182	4	9	-18	156	6	1	2	54	13	5*
18	20	49	12*	-10	368	8	-3	5	596	12	12	-17	67	13	1*	3	250	6	-0
19	60	21	-5*	-9	23	27	-0*	6	67	6	-5	-16	176	5	-5	4	20	30	2*
20	12	40	-27*	-8	274	6	5	7	543	11	-6	-15	39	41	-22*	5	178	5	-2
H,K=		1,	2	-7	133	4	5	8	53	11	-17*	-14	93	7	0	6	85	7	7
-20	81	19	-7*	-6	21	25	3*	9	287	6	10	-13	0	33	-37*	7	128	8	4
-19	140	10	5	-5	51	11	17*	10	55	11	3*	-12	25	45	-15*	8	40	43	8*
-18	123	12	-3	-4	260	5	-3	11	21	32	-7*	-11	0	47	-15*	9	287	6	-3
-17	176	6	8	-3	279	6	22	12	0	38	-5*	-10	159	5	1	10	41	41	16*
-16	138	6	-11	-2	605	12	35	13	108	8	4	-9	131	5	6	11	259	6	-3
-15	183	6	-6	-1	204	5	14	14	48	23	-12*	-8	242	5	-1	12	42	15	27*
-14	120	6	-5	0	696	14	31	15	175	7	-2	-7	139	5	-3	13	201	5	-0
-13	105	6	4	1	226	5	13	16	27	35	-4*	-6	328	7	3	14	8	34	-7*
-12	103	12	-1	2	975	20	48	17	209	6	3	-5	187	5	2	15	151	8	7
-11	59	8	6	3	283	6	18	18	53	19	30*	-4	355	7	-4	16	0	36	-12*
-10	181	4	1	4	356	7	5	19	154	8	7	-3	150	5	-10	H,K=		1,	8
-9	341	8	-8	5	57	16	10*	H,K=		1,	5	-2	160	5	5	-15	38	27	-20*
-8	344	7	-3	6	70	4	4	-19	30	37	3*	-1	79	5	-1	-14	102	10	4
-7	551	11	5	7	25	20	17*	-18	53	17	38*	0	21	26	-14*	-13	29	46	4*
-6	403	8	3	8	181	4	-6	-17	34	41	-14*	1	74	5	-2	-12	50	13	29*
-5	416	9	-14	9	84	7	2	-16	70	9	9	2	129	4	-2	-11	39	18	13*
-4	289	7	7	10	312	7	-2	-15	104	12	0	3	76	6	-1	-10	68	8	-5
-3	64	10	25	11	88	7	-7	-14	171	6	-5	4	318	7	-6	-9	85	10	-6
-2	323	7	-11	12	404	9	-12	-13	125	15	-2	5	125	5	3	-8	221	5	-1
-1	269	6	-1	13	64	11	-11	-12	236	6	-4	6	336	7	7	-7	128	5	3
0	183	5	9	14	289	8	4	-11	221	7	-3	7	193	6	-5	-6	355	8	-7
1	307	7	5	15	34	35	-8*	-10	240	5	-3	8	278	6	0	-5	132	5	-8
2	50	5	30	16	124	6	1	-9	168	5	-11	9	78	7	-5	-4	303	7	-5
3	382	8	20	17	30	36	18*	-8	229	5	-7	10	186	5	1	-3	101	9	-3
4	526	11	34	18	41	29	31*	-7	30	19	14*	11	31	41	1*	-2	143	5	-3
5	739	15	23	19	0	54	-16*	-6	117	6	1	12	32	32	14*	-1	86	9	-4
6	458	9	5	20	73	12	-14	-5	27	20	-10*	13	16	42	0*	0	34	38	4*
7	569	12	7	H,K=		1,	4	-4	201	5	-5	14	115	6	7	1	0	31	-7*
8	341	7	14	-19	149	9	-3	-3	146	4	-2	15	0	35	-43*	2	178	5	0
9	237	5	5	-18	11	39	-19*	-2	482	10	5	16	169	6	-5	3	91	6	9
10	9	29	-27*	-17	220	6	-1	-1	439	9	-1	17	60	13	-5*	4	322	7	-2
11	45	14	5*	-16	49	29	-6*	0	451	9	12	H,K=		1,	7	5	159	7	-1
12	42	19	-18*	-15	207	5	-3	1	277	6	-7	-17	25	36	-9*	6	338	7	-3
13	109	7	-5	-14	80	11	5	2	289	6	5	-16	33	40	2*	7	131	7	-8
14	74	12	0	-13	120	7	4	3	151	4	-7	-15	126	10	-8	8	194	5	-8
15	151	6	-0	-12	46	13	27*	4	124	4	-1	-14	24	35	15*	9	69	9	-8
16	112	9	-6	-11	89	6	8	5	35	21	18*	-13	204	6	0	10	85	7	8
17	159	6	-6	-10	43	12	1*	6	22	33	16*	-12	32	32	12*	11	40	27	13*
18	122	8	-4	-9	300	6	0	7	35	19	12*	-11	274	7	-3	12	34	27	13*
19	136	9	-0	-8	128	5	2	8	184	7	-6	-10	0	33	-13*	13	30	34	22*
20	95	10	14	-7	527	11	16	9	137	5	-1	-9	266	6	1	14	103	10	10
H,K=		1,	3	-6	174	4	3	10	273	6	1	-8	47	12	30*	15	74	8	21
-20	55	17	-7*	-5	454	11	7	11	167	6	5	-7	112	5	13	H,K=		1,	9
-19	32	38	6*	-4	69	4	6	12	256	7	-1	-6	0	31	-18*	-13	114	6	-1
-18	35	35	26*	-3	505	10	-1	13	158	7	2	-5	83	6	1	-12	150	6	-1
-17	35	37	27*	-2	89	8	-1	14	156	6	5	-4	15	30	-10*	-11	109	6	-2

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2 PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	133	8	-6	1	41	43	5*	5	728	24	7	19	0	43	-38*	-8	0	31	-7*
-9	82	11	2	2	174	6	4	6	360	12	9	20	59	17	-4*	-7	209	5	6
-8	97	9	6	3	45	29	10*	7	564	12	-1	H,K=	2,	3		-6	104	4	-0
-7	65	15	6*	4	86	7	-3	8	224	5	-0	-20	137	7	-2	-5	147	4	-5
-6	13	37	2*	5	0	35	-34*	9	304	6	-0	-19	20	50	-8*	-4	51	5	-12
-5	0	31	-11*	6	27	34	15*	10	157	5	-6	-18	196	5	8	-3	451	9	1
-4	123	6	-3	7	51	12	39*	11	32	37	2*	-17	93	10	-10	-2	57	5	3
-3	105	5	-7	H,K=	2,	0		12	52	17	-3*	-16	234	7	-9	-1	635	13	-18
-2	161	5	0	-20	106	9	-4	13	104	9	-3	-15	68	14	-2*	0	135	4	-0
-1	226	5	2	-18	19	36	13*	14	69	18	-1*	-14	184	8	-2	1	565	12	-6
0	173	5	-6	-16	103	10	-1	15	199	9	1	-13	10	38	-13*	2	174	4	-2
1	190	5	-0	-14	220	5	3	16	104	7	5	-12	37	17	6*	3	365	7	-1
2	177	5	4	-12	503	11	9	17	190	6	3	-11	22	30	14*	4	26	13	5*
3	108	5	7	-10	506	10	-2	18	67	13	-17*	-10	255	6	-1	5	59	5	-6
4	146	5	-3	-8	393	8	1	19	174	6	3	-9	41	10	8*	6	79	5	-2
5	69	9	15	-6	156	5	-4	20	71	19	-3*	-8	491	10	7	7	107	6	-2
6	28	32	-12*	-4	400	8	12	H,K=	2,	2	-7	106	4	-3		8	23	29	-17*
7	38	16	21*	-2	1080	22	-137	-20	57	17	6*	-6	585	12	11	9	307	7	2
8	91	9	10	0	1110	27	-38	-19	73	23	20*	-5	130	5	-9	10	23	38	-23*
9	98	10	-5	2	517	11	3	-18	36	42	15*	-4	458	9	-5	11	413	9	-7
10	129	7	-9	4	163	10	16	-17	37	43	2*	-3	202	4	19	12	117	13	9
11	141	5	10	6	83	10	14	-16	89	8	15	-2	391	8	13	13	292	7	-3
12	139	9	-2	8	315	7	0	-15	137	12	6	-1	132	6	16	14	93	8	-5
13	122	8	7	10	390	9	-6	-14	138	6	-1	0	128	5	-6	15	159	7	4
H,K=	1,	10		12	417	9	2	-13	310	7	6	1	18	21	-0*	16	32	38	-11*
-11	35	40	2*	14	329	7	3	-12	259	6	3	2	267	6	7	17	54	14	15*
-10	27	34	16*	16	75	9	9	-11	359	7	-2	3	22	23	11*	18	32	37	24*
-9	107	9	-4	18	69	13	31	-10	270	6	-3	4	739	15	-8	19	50	18	-9*
-8	36	22	-0*	20	88	14	4	-9	363	8	1	5	129	3	1	H,K=	2,	5	
-7	173	7	-4	H,K=	2,	1		-8	54	7	-15	6	655	13	-1	-19	108	8	1
-6	46	15	-3*	-21	102	8	-1	-7	88	4	4	7	15	25	-10*	-18	152	7	2
-5	205	7	-6	-20	77	12	9	-6	65	7	22	8	333	7	0	-17	122	6	-1
-4	33	42	26*	-19	182	6	1	-5	184	5	3	9	118	4	1	-16	148	6	-8
-3	176	6	-1	-18	127	6	-3	-4	84	8	15	10	116	6	5	-15	94	7	-9
-2	46	12	41*	-17	199	5	1	-3	373	8	9	11	35	36	-8*	-14	85	9	-6
-1	50	13	0*	-16	101	12	-1	-2	360	7	23	12	31	34	-9*	-13	68	9	3
0	31	35	6*	-15	178	8	2	-1	151	4	-10	13	35	36	17*	-12	21	39	3*
1	84	7	-8	-14	100	6	3	0	287	6	-11	14	117	17	-17	-11	22	34	-2*
2	49	11	36*	-13	136	5	-6	1	701	14	27	15	0	43	-12*	-10	108	5	-3
3	162	6	1	-12	41	14	-4*	2	83	12	-20	16	174	6	0	-9	189	5	6
4	50	26	9*	-11	47	35	-6*	3	601	12	34	17	40	41	-13*	-8	263	6	0
5	188	5	3	-10	61	11	-2	4	377	10	15	18	172	6	-7	-7	248	6	-5
6	34	26	-0*	-9	300	16	-0	5	60	6	-6	19	6	41	-39*	-6	305	6	-2
7	168	5	-8	-8	132	4	-4	6	39	8	-7*	H,K=	2,	4		-5	333	7	2
8	23	41	-13*	-7	649	16	-24	7	173	4	2	-20	0	49	-10*	-4	338	7	-10
9	124	6	4	-6	127	5	-21	8	117	7	-3	-19	34	36	-6*	-3	275	6	-5
10	45	21	22*	-5	601	12	32	9	110	4	-1	-18	0	36	-24*	-2	264	6	-6
H,K=	1,	11		-4	389	8	32	10	279	6	-7	-17	9	35	-4*	-1	76	4	7
-7	31	34	12*	-3	231	6	8	11	237	6	-6	-16	38	30	19*	0	7	24	-14*
-6	19	34	8*	-2	50	15	-47*	12	237	6	-1	-15	173	5	-2	1	46	7	-7
-5	42	19	19*	-1	283	7	-10	13	295	7	-2	-14	28	42	20*	2	311	7	-13
-4	98	7	2	0	241	6	-21	14	213	12	1	-13	298	7	-2	3	80	4	10
-3	59	11	5*	1	17	30	0*	15	160	11	-11	-12	57	11	-10*	4	286	6	-7
-2	189	5	2	2	155	6	4	16	109	8	19	-11	352	8	1	5	301	6	2
-1	59	10	11	3	616	18	20	17	70	13	17	-10	103	5	2	6	353	7	7
0	191	7	-8	4	26	52	-20*	18	0	50	-17*	-9	311	7	5	7	281	6	-1

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	308	7	5	-10	40	17	-0*	13	78	14	14	-5	58	11	-6*	0	102	10	-4
9	189	5	1	-9	195	6	-4	14	145	6	-3	-4	188	5	7	1	545	19	-20
10	155	6	1	-8	35	35	7*	H,K=		2,	9	-3	54	11	7*	2	281	7	7
11	65	9	20	-7	296	6	-6	-13	36	38	-4*	-2	114	7	-5	3	463	20	27
12	16	50	5*	-6	32	33	8*	-12	30	34	29*	-1	18	43	4*	4	42	24	6*
13	31	38	-15*	-5	365	8	-4	-11	47	36	-7*	0	44	20	39*	5	206	10	-3
14	94	7	2	-4	13	30	-6*	-10	81	8	-2	1	39	18	18*	6	82	6	10
15	82	8	-3	-3	331	7	5	-9	103	6	-1	2	64	10	-14	7	71	6	-7
16	157	5	-5	-2	27	31	16*	-8	153	6	3	3	63	9	25	8	136	5	-0
17	132	6	21	-1	118	5	8	-7	144	5	-2	4	143	8	-7	9	378	8	-0
18	154	8	0	0	6	29	-10*	-6	185	5	10	5	51	12	24*	10	102	9	-7
H,K=		2,	6	1	93	5	4	-5	176	6	-2	6	179	6	3	11	341	8	11
-18	41	25	11*	2	37	15	10*	-4	186	5	-1	H,K=		3,	0	12	156	6	-1
-17	30	35	10*	3	289	7	5	-3	138	5	4	-20	175	7	2	13	345	8	6
-16	84	14	-0	4	0	31	-8*	-2	138	5	0	-18	257	6	5	14	116	17	-3
-15	52	18	-3*	5	393	8	-1	-1	46	12	9*	-16	174	5	4	15	201	7	10
-14	178	5	-1	6	33	23	29*	0	20	31	8*	-14	203	6	3	16	21	42	-20*
-13	134	5	-1	7	352	7	-4	1	68	8	-3	-12	29	31	3*	17	17	40	-8*
-12	228	6	-1	8	27	41	-14*	2	162	5	2	-10	253	6	-2	18	38	39	37*
-11	115	9	-2	9	192	5	3	3	127	5	2	-8	456	10	-6	19	52	19	4*
-10	336	7	1	10	46	15	19*	4	164	5	-3	-6	850	17	3	20	25	40	6*
-9	102	10	14	11	42	16	-7*	5	134	5	-2	-4	740	15	-15	H,K=		3,	2
-8	259	6	-1	12	0	33	-11*	6	169	5	-2	-2	175	7	-8	-20	104	8	2
-7	47	10	14*	13	31	34	-18*	7	121	5	-8	0	81	11	9	-19	166	6	11
-6	52	10	-6*	14	29	34	23*	8	149	6	-5	2	179	5	8	-18	119	8	9
-5	27	28	2*	15	135	7	9	9	90	12	-0	4	574	12	14	-17	191	23	10
-4	188	5	4	16	7	37	-5*	10	57	19	-6*	6	692	15	3	-16	172	7	-2
-3	192	5	2	H,K=		2,	8	11	18	36	-13*	8	653	13	5	-15	115	7	-6
-2	445	9	0	-15	37	44	-5*	12	0	36	-2*	10	187	5	-7	-14	136	5	-10
-1	212	5	-2	-14	150	8	-7	13	6	39	-19*	12	24	35	19*	-13	121	5	-1
0	460	9	4	-13	90	12	-6	H,K=		2,	10	14	193	6	-3	-12	31	37	-5*
1	189	4	5	-12	188	5	2	-11	147	6	1	16	242	6	-4	-11	37	14	24*
2	301	6	-2	-11	103	9	1	-10	42	20	21*	18	205	6	7	-10	158	4	-1
3	0	29	-31*	-10	182	7	3	-9	141	6	9	20	162	10	14	-9	216	6	0
4	228	5	-7	-9	77	7	-9	-8	32	34	16*	H,K=		3,	1	-8	248	5	-2
5	117	8	-1	-8	143	9	5	-7	101	6	1	-21	119	10	1	-7	407	8	-0
6	42	15	-15*	-7	30	40	25*	-6	24	34	19*	-20	47	18	-13*	-6	314	7	-2
7	0	31	-11*	-6	36	43	22*	-5	25	34	6*	-19	89	8	-1	-5	441	9	-18
8	135	5	-1	-5	96	6	-1	-4	36	20	9*	-18	39	20	7*	-4	355	10	5
9	134	5	6	-4	154	6	0	-3	166	5	6	-17	76	10	2	-3	530	13	51
10	241	6	-14	-3	102	11	-2	-2	35	22	11*	-16	86	7	3	-2	254	6	5
11	146	5	-3	-2	239	5	-3	-1	233	6	1	-15	172	5	1	-1	158	8	5
12	227	7	4	-1	93	6	2	0	71	8	15	-14	89	7	-9	0	96	10	18
13	98	6	6	0	303	7	0	1	220	5	1	-13	292	6	-2	1	21	41	3*
14	160	5	4	1	149	5	-3	2	77	7	22	-12	134	5	-1	2	112	7	-1
15	23	37	-20*	2	267	6	-2	3	162	5	-1	-11	471	16	-19	3	207	5	-23
16	94	7	10	3	108	10	-2	4	28	34	24*	-10	128	5	-3	4	416	11	3
17	0	39	-4*	4	139	7	-7	5	59	21	-8*	-9	420	9	-2	5	514	15	-11
H,K=		2,	7	5	21	31	8*	6	28	33	-8*	-8	247	6	9	6	332	7	-6
-17	159	10	1	6	48	13	16*	7	30	34	1*	-7	0	30	-29*	7	486	15	-7
-16	16	35	2*	7	47	12	2*	8	36	23	29*	-6	57	12	24*	8	180	5	-0
-15	162	5	-0	8	142	6	2	9	120	6	-7	-5	324	7	30	9	151	5	-7
-14	0	35	-7*	9	84	7	13	10	43	17	23*	-4	284	7	12	10	74	8	-12
-13	60	19	-19*	10	219	5	1	H,K=		2,	11	-3	349	8	-10	11	50	17	15*
-12	39	19	-5*	11	84	10	0	-7	54	12	12*	-2	390	8	8	12	40	43	20*
-11	60	9	4	12	203	5	-2	-6	183	5	-5	-1	653	22	-24	13	50	18	13*

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
14	69	38	9*	-13	75	10	8	3	204	5	-3	-15	128	6	10	8	188	5	5
15	120	9	-16	-12	48	13	0*	4	95	6	-4	-14	28	34	22*	9	91	6	4
16	99	8	3	-11	57	9	12	5	211	5	1	-13	242	6	1	10	80	8	1
17	162	7	1	-10	72	13	-2	6	28	29	4*	-12	0	33	-20*	11	34	36	14*
18	130	8	0	-9	302	7	1	7	55	9	1	-11	254	6	-3	12	12	34	7*
19	117	12	-7	-8	153	4	2	8	138	5	-7	-10	17	31	14*	13	21	34	-6*
20	78	11	2	-7	460	9	9	9	142	5	3	-9	205	7	0	14	80	8	7
H,K=		3,	3	-6	144	5	6	10	294	7	-7	-8	36	36	-2*	H,K=		3,	9
-20	102	8	8	-5	590	12	-9	11	167	6	2	-7	101	6	3	-13	95	8	-15
-19	30	50	8*	-4	66	4	5	12	255	6	-7	-6	25	39	12*	-12	168	7	3
-18	26	36	-12*	-3	431	9	8	13	161	5	-3	-5	53	18	5*	-11	111	7	3
-17	41	18	10*	-2	47	10	-3*	14	111	8	2	-4	67	7	-4	-10	141	6	2
-16	86	7	5	-1	210	5	8	15	107	10	-9	-3	266	6	0	-9	76	14	3*
-15	73	9	-7	0	0	27	-15*	16	80	8	15	-2	52	14	-0*	-8	109	6	0
-14	290	8	-3	1	300	6	11	17	48	53	18*	-1	382	8	2	-7	72	12	-6
-13	72	8	6	2	120	3	1	18	19	38	12*	0	32	32	-0*	-6	43	22	25*
-12	354	8	7	3	490	10	12	H,K=		3,	6	1	343	7	-2	-5	20	33	15*
-11	0	30	-22*	4	83	7	10	-18	144	6	-5	2	31	21	3*	-4	87	6	2
-10	404	8	5	5	575	12	14	-17	65	11	-15	3	274	6	-5	-3	122	6	0
-9	99	6	7	6	108	4	2	-16	170	5	-8	4	40	14	14*	-2	166	5	-5
-8	312	7	3	7	446	10	1	-15	78	8	-9	5	117	6	-0	-1	210	5	-0
-7	83	4	10	8	90	9	-7	-14	99	6	0	6	34	37	-29*	0	206	7	-6
-6	122	3	4	9	289	6	2	-13	44	15	-25*	7	100	6	5	1	194	5	-13
-5	22	44	-16*	10	33	26	0*	-12	33	35	26*	8	33	42	15*	2	194	6	0
-4	260	5	-3	11	83	12	8	-11	37	44	-8*	9	221	6	-7	3	135	5	0
-3	35	19	25*	12	45	16	25*	-10	105	8	9	10	0	32	-4*	4	110	5	6
-2	331	7	-19	13	84	9	-9	-9	124	5	7	11	247	6	0	5	32	38	3*
-1	140	4	-8	14	8	53	-19*	-8	262	6	-5	12	48	15	39*	6	52	10	3*
0	696	17	3	15	156	5	-3	-7	162	5	-4	13	194	5	-3	7	36	26	-12*
1	57	6	-9	16	35	37	24*	-6	340	8	-2	14	0	40	-9*	8	63	9	13
2	710	17	17	17	200	6	-2	-5	158	4	-5	15	115	7	-6	9	111	6	-1
3	109	4	14	18	0	39	-9*	-4	335	7	6	16	9	36	7*	10	137	6	-8
4	354	7	5	19	153	6	2	-3	174	4	9	H,K=		3,	8	11	123	7	1
5	45	6	-3	H,K=		3,	5	-2	211	5	4	-15	48	16	-6*	12	151	6	7
6	51	6	11	-19	33	48	8*	-1	105	5	0	-14	105	9	-6	H,K=		3,	10
7	41	10	5*	-18	36	42	25*	0	25	30	-5*	-13	41	41	13*	-11	32	34	0*
8	154	4	4	-17	0	42	-28*	1	25	34	-0*	-12	47	14	30*	-10	37	20	19*
9	41	25	-7*	-16	46	35	-13*	2	127	4	-0	-11	17	34	-27*	-9	123	6	-2
10	343	7	1	-15	97	7	2	3	153	4	1	-10	104	6	2	-8	46	19	-11*
11	123	5	-2	-14	199	6	0	4	273	6	-4	-9	83	7	16	-7	180	5	-12
12	392	8	-5	-13	138	8	0	5	97	11	-6	-8	208	5	-3	-6	48	14	-2*
13	50	15	-1*	-12	255	7	-6	6	351	7	-4	-7	117	7	6	-5	207	5	1
14	246	6	-2	-11	256	6	-1	7	122	5	3	-6	286	6	-5	-4	45	13	27*
15	37	38	26*	-10	237	5	-4	8	280	6	-5	-5	126	5	2	-3	157	8	-2
16	110	7	7	-9	222	5	-2	9	91	6	-2	-4	246	6	-5	-2	41	15	17*
17	47	19	30*	-8	181	5	1	10	168	6	-6	-3	155	5	-0	-1	63	10	9
18	14	40	-2*	-7	62	7	3	11	62	26	-2*	-2	191	5	3	0	58	18	37*
19	0	41	-5*	-6	16	27	-1*	12	45	13	38*	-1	110	5	-5	1	65	9	-7
H,K=		3,	4	-5	80	5	-1	13	0	33	-5*	0	38	45	-1*	2	30	41	10*
-20	59	13	9*	-4	291	6	9	14	107	8	5	1	31	39	14*	3	144	6	-6
-19	168	6	-2	-3	271	6	5	15	54	16	-7*	2	201	5	3	4	55	11	9*
-18	77	19	22*	-2	465	10	14	16	129	6	-10	3	147	5	-6	5	173	7	-1
-17	195	6	3	-1	299	6	6	17	73	11	-8	4	314	7	-3	6	26	34	-20*
-16	37	22	-2*	0	491	10	3	H,K=		3,	7	5	122	6	-0	7	174	5	0
-15	210	5	4	1	141	4	-3	-17	33	35	22*	6	241	6	-8	8	51	13	8*
-14	38	22	11*	2	321	7	10	-16	38	21	30*	7	102	6	-9	9	128	11	-9

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	37	24	8*	-3	514	11	22	12	255	6	-0	-13	304	7	-3	4	300	7	4
H,K=		3,	11	-2	109	10	-7	13	244	8	-4	-12	48	13	-12*	5	280	6	3
-7	46	15	29*	-1	218	6	14	14	181	9	-1	-11	302	8	-6	6	337	7	2
-6	35	26	17*	0	110	12	41	15	184	7	-7	-10	104	10	-3	7	251	6	-4
-5	31	35	10*	1	72	16	-11*	16	59	16	-6*	-9	330	8	-5	8	252	6	-5
-4	82	17	-1*	2	91	11	3	17	47	21	4*	-8	9	28	-7*	9	149	5	-2
-3	29	41	-14*	3	491	19	12	18	49	26	49*	-7	187	5	0	10	160	5	1
-2	174	5	3	4	121	5	-2	19	37	41	-9*	-6	39	9	16*	11	66	14	13*
-1	59	10	14	5	522	14	-7	H,K=		4,	3	-5	110	4	-1	12	0	42	-3*
0	185	5	-10	6	258	6	2	-20	127	7	-9	-4	28	13	5*	13	51	17	16*
1	59	9	20	7	540	11	9	-19	20	36	-25*	-3	435	9	4	14	115	8	5
2	156	5	-1	8	295	6	7	-18	194	6	-1	-2	17	24	-31*	15	78	10	-4
3	46	18	18*	9	286	7	-4	-17	45	24	0*	-1	514	10	0	16	154	6	8
4	95	12	5	10	119	6	-4	-16	216	6	-9	0	209	5	-12	17	94	8	2
5	30	38	14*	11	58	13	1*	-15	92	8	-2	1	564	11	-4	H,K=		4,	6
6	0	36	-11*	12	33	38	27*	-14	159	11	0	2	101	4	3	-18	26	35	15*
H,K=		4,	0	13	87	12	5	-13	23	37	19*	3	324	7	-11	-17	44	49	30*
-20	130	7	-3	14	66	30	13*	-12	20	32	-1*	4	91	6	4	-16	86	8	14
-18	62	11	4	15	173	6	-1	-11	40	20	17*	5	119	4	-2	-15	49	15	-8*
-16	173	6	-1	16	110	9	4	-10	163	5	-7	6	62	8	4	-14	174	6	4
-14	233	5	5	17	186	7	0	-9	112	5	1	7	101	5	2	-13	119	9	-1
-12	409	9	-10	18	76	12	-6	-8	451	10	-6	8	35	18	-5*	-12	252	9	-4
-10	398	8	-3	19	143	9	-1	-7	149	4	-3	9	256	6	-7	-11	147	5	-13
-8	405	8	-7	H,K=		4,	2	-6	578	12	6	10	100	6	-5	-10	292	8	-2
-6	162	4	11	-20	81	9	1	-5	53	7	3	11	370	13	-8	-9	59	9	9
-4	170	8	-41	-19	98	7	0	-4	605	13	5	12	92	27	10*	-8	200	7	-2
-2	550	11	-41	-18	33	43	15*	-3	135	3	-2	13	255	6	-3	-7	54	9	-3
0	575	12	-37	-17	0	43	-27*	-2	372	8	-2	14	86	8	-1	-6	9	30	-20*
2	685	14	43	-16	39	23	-10*	-1	27	33	0*	15	118	7	-8	-5	22	29	-4*
4	229	6	-12	-15	239	6	-5	0	88	5	16	16	42	42	20*	-4	132	4	-2
6	64	11	-2	-14	221	6	-8	1	40	9	25*	17	39	31	-1*	-3	80	5	3
8	317	7	13	-13	263	6	-8	2	445	12	5	18	30	42	6*	-2	386	8	-3
10	406	9	19	-12	241	6	-2	3	44	10	-0*	H,K=		4,	5	-1	199	5	-2
12	335	8	9	-11	294	6	2	4	451	12	5	-19	109	7	-4	0	386	8	4
14	256	6	2	-10	206	5	2	5	92	4	-3	-18	106	9	-17	1	191	5	-1
16	104	8	16	-9	320	7	1	6	454	9	-10	-17	106	7	-2	2	290	7	2
18	32	41	2*	-8	102	4	2	7	80	5	5	-16	139	6	1	3	105	6	8
H,K=		4,	1	-7	199	5	4	8	338	12	-10	-15	113	7	-6	4	239	6	-2
-21	108	7	8	-6	14	25	-24*	9	67	8	9	-14	153	7	-3	5	67	7	10
-20	60	13	-3*	-5	288	6	25	10	192	6	1	-13	33	33	5*	6	45	24	11*
-19	171	6	4	-4	111	6	-10	11	66	16	-7*	-12	53	36	-4*	7	38	17	32*
-18	124	8	2	-3	431	9	30	12	45	26	31*	-11	40	42	33*	8	167	6	3
-17	196	6	-0	-2	484	12	12	13	32	47	23*	-10	127	7	-5	9	89	7	-2
-16	102	8	-10	-1	411	10	1	14	113	8	4	-9	137	5	4	10	217	7	-0
-15	153	6	-7	0	506	15	34	15	0	38	-35*	-8	256	7	-8	11	122	5	-6
-14	49	13	27*	1	468	15	-9	16	180	6	5	-7	247	5	0	12	233	6	-0
-13	172	5	-4	2	428	12	30	17	50	19	4*	-6	311	7	-8	13	81	9	5
-12	68	10	9	3	401	12	-6	18	173	8	3	-5	315	7	-4	14	156	6	1
-11	0	33	-11*	4	304	11	7	19	54	19	3*	-4	295	7	-1	15	24	40	-23*
-10	26	35	-10*	5	119	4	-7	H,K=		4,	4	-3	229	5	-7	16	64	16	-2*
-9	304	7	8	6	41	9	13*	-19	60	12	0*	-2	198	5	5	H,K=		4,	7
-8	192	5	2	7	91	5	-13	-18	0	36	-8*	-1	84	4	-4	-17	154	7	2
-7	553	14	3	8	173	5	-5	-17	21	51	6*	0	69	5	1	-16	14	40	11*
-6	364	10	-9	9	206	6	5	-16	15	35	-17*	1	0	27	-21*	-15	166	11	-5
-5	550	17	4	10	227	6	-2	-15	141	5	-7	2	146	4	-3	-14	14	38	7*
-4	154	6	-32	11	256	6	-4	-14	45	14	0*	3	101	4	-0	-13	93	7	3

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	44	31	7*	12	183	6	2	-2	108	7	10	5	95	5	6	H,K=		5,	3
-11	70	12	-18	13	72	14	-3*	-1	44	18	27*	6	88	5	-2	-20	124	8	1
-10	25	43	-5*	14	133	6	2	0	17	33	-5*	7	151	5	6	-19	26	38	14*
-9	173	8	-6	H,K=		4,	9	1	0	44	-8*	8	36	19	-15*	-18	72	9	11
-8	48	18	5*	-13	61	13	17*	2	66	12	9	9	280	7	10	-17	38	23	5*
-7	304	8	-9	-12	25	37	17*	3	36	22	6*	10	144	6	-6	-16	118	5	16
-6	20	36	6*	-11	31	34	1*	4	152	6	4	11	303	7	2	-15	29	49	22*
-5	374	8	-2	-10	94	10	-6	5	22	40	-15*	12	135	8	1	-14	299	9	-7
-4	57	12	20*	-9	102	10	1	H,K=		5,	0	13	293	7	-3	-13	74	8	-4
-3	312	7	-3	-8	138	6	3	-20	136	8	4	14	110	12	2	-12	309	7	7
-2	34	42	17*	-7	138	8	-6	-18	189	5	5	15	170	6	7	-11	92	6	7
-1	131	5	5	-6	174	5	1	-16	254	8	-5	16	83	10	3	-10	305	6	10
0	30	37	9*	-5	152	5	1	-14	186	6	-3	17	47	34	9*	-9	178	4	-4
1	86	6	4	-4	193	5	3	-12	90	6	1	18	25	40	17*	-8	347	7	4
2	19	31	-9*	-3	81	9	5	-10	248	6	0	19	59	17	12*	-7	49	7	-2
3	328	7	-3	-2	125	5	-3	-8	446	9	-5	H,K=		5,	2	-6	162	4	6
4	28	37	21*	-1	33	44	-8*	-6	652	13	-35	-20	66	12	-7*	-5	88	4	10
5	401	9	-10	0	37	16	35*	-4	575	13	-17	-19	124	7	-0	-4	169	4	-2
6	39	19	9*	1	35	18	21*	-2	241	6	-8	-18	124	8	1	-3	54	5	-3
7	302	7	-6	2	110	11	1	0	51	28	1*	-17	191	6	1	-2	404	8	-10
8	28	32	18*	3	94	7	-4	2	436	9	27	-16	152	9	1	-1	279	6	13
9	188	6	4	4	163	5	0	4	563	14	10	-15	169	8	-10	0	635	13	-6
10	34	34	21*	5	120	5	1	6	505	10	12	-14	160	8	-4	1	94	3	3
11	87	7	16	6	166	5	7	8	505	11	12	-13	95	9	3	2	483	13	1
12	0	34	-5*	7	109	6	3	10	198	6	7	-12	34	34	-0*	3	60	6	11
13	46	17	-8*	8	135	9	-1	12	59	22	9*	-11	21	32	-1*	4	255	6	-9
14	24	42	8*	9	84	11	-3	14	174	7	0	-10	81	6	-1	5	106	5	-13
15	128	7	5	10	67	12	-10	16	194	7	-4	-9	190	5	-4	6	16	27	-7*
H,K=		4,	8	11	23	35	-3*	18	195	8	5	-8	294	6	1	7	26	34	8*
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-14	118	8	-4	H,K=		4,	10	-21	118	8	-8	-6	291	6	-8	9	8	38	-33*
-13	104	6	2	-10	22	35	-14*	-20	31	36	-15*	-5	571	15	9	10	360	8	-8
-12	207	6	3	-9	150	6	-2	-19	89	8	-1	-4	312	6	-16	11	75	9	-2
-11	117	6	3	-8	41	17	15*	-18	52	20	5*	-3	371	10	9	12	319	7	-10
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-9	75	8	-2	-6	31	32	30*	-16	97	7	-0	-1	290	6	31	14	215	6	-5
-8	112	6	2	-5	56	17	15*	-15	191	6	-6	0	17	31	-11*	15	13	38	-0*
-7	21	33	3*	-4	17	35	12*	-14	165	5	-9	1	22	26	11*	16	80	11	-16
-6	40	14	14*	-3	141	7	-3	-13	300	7	-7	2	187	5	3	17	16	53	-5*
-5	69	10	10	-2	43	17	20*	-12	115	6	-3	3	272	6	-15	18	28	40	9*
-4	112	8	-5	-1	210	6	-6	-11	358	8	-11	4	284	6	-3	H,K=		5,	4
-3	70	13	-3*	0	49	20	-11*	-10	157	6	-4	5	438	15	-7	-19	149	6	-4
-2	269	6	1	1	233	6	1	-9	256	6	-7	6	324	7	2	-18	34	36	-9*
-1	100	13	8	2	33	47	-7*	-8	200	5	10	7	363	8	-6	-17	163	7	-2
0	332	7	-3	3	155	5	-4	-7	160	4	-3	8	208	5	-6	-16	36	41	4*
1	127	5	3	4	10	40	-6*	-6	63	6	-1	9	240	6	-2	-15	185	5	2
2	275	6	-7	5	45	22	-22*	-5	36	23	-11*	10	114	7	-3	-14	28	32	11*
3	74	8	2	6	0	34	-17*	-4	233	6	6	11	90	10	1	-13	143	7	5
4	142	5	1	7	36	37	11*	-3	568	17	50	12	48	20	5*	-12	27	38	17*
5	22	32	9*	8	18	43	12*	-2	264	6	3	13	38	47	12*	-11	65	9	-5
6	0	37	-17*	9	130	6	1	-1	582	18	23	14	27	49	-29*	-10	46	15	9*
7	10	39	-14*	H,K=		4,	11	0	368	15	11	15	138	6	15	-9	287	6	-8
8	127	5	0	-6	172	6	-2	1	538	16	-23	16	113	7	10	-8	51	9	3
9	41	43	-0*	-5	51	13	10*	2	352	10	11	17	166	10	1	-7	433	9	-4
10	187	6	-0	-4	158	6	1	3	406	12	-14	18	115	14	-0	-6	65	7	-5
11	79	9	-13	-3	30	34	1*	4	202	5	9	19	120	10	2	-5	414	9	0

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	144	4	2	13	153	5	-5	-2	9	30	8*	-6	33	24	29*	-8	185	4	-20
-3	373	8	4	14	126	6	-2	-1	385	8	-6	-5	39	18	26*	-6	342	7	-3
-2	53	6	11	15	101	7	2	0	16	34	12*	-4	85	7	-3	-4	221	5	7
-1	192	4	7	16	66	11	11	1	331	7	-3	-3	130	8	-2	-2	712	14	22
0	109	4	-5	17	37	37	18*	2	11	35	-17*	-2	141	5	-5	0	377	8	-37
1	135	5	-3	H,K=		5,	6	3	265	6	-4	-1	171	5	-2	2	503	10	-22
2	172	5	8	-18	145	9	-2	4	36	37	20*	0	200	6	3	4	365	8	-4
3	368	8	12	-17	85	8	-0	5	118	7	-8	1	165	5	-5	6	35	21	-7*
4	48	10	-3*	-16	170	5	-4	6	20	48	13*	2	184	6	0	8	301	7	9
5	518	11	1	-15	86	8	-1	7	64	13	5*	3	89	7	2	10	347	8	1
6	30	20	8*	-14	141	6	-9	8	46	22	44*	4	96	12	-1	12	337	7	2
7	402	9	-4	-13	76	8	0	9	180	5	4	5	29	38	20*	14	223	6	7
8	64	11	5	-12	20	36	-0*	10	18	33	11*	6	32	33	-1*	16	104	8	1
9	257	7	-2	-11	27	35	-9*	11	212	6	-2	7	47	13	8*	18	41	22	41*
10	43	16	-7*	-10	124	13	-1	12	46	14	34*	8	64	10	1	H,K=		6,	1
11	64	22	-9*	-9	168	6	-0	13	205	6	-3	9	96	7	8	-20	68	11	4
12	38	47	26*	-8	282	6	-3	14	0	40	-14*	10	136	6	-6	-19	132	6	-6
13	71	9	2	-7	127	5	-1	15	120	9	6	11	109	8	-4	-18	72	11	-2
14	0	45	-6*	-6	362	8	-2	H,K=		5,	8	H,K=		5,	10	-17	175	5	-5
15	169	6	1	-5	126	5	2	-15	48	15	12*	-10	0	46	-24*	-16	118	6	-19
16	26	44	6*	-4	360	8	4	-14	87	9	-10	-9	134	9	-5	-15	221	7	-7
17	165	9	-1	-3	113	5	6	-13	53	12	14*	-8	58	12	-3*	-14	75	14	-5
18	14	41	-11*	-2	287	7	-3	-12	0	44	-31*	-7	189	6	-0	-13	146	6	-5
H,K=		5,	5	-1	74	6	5	-11	25	35	7*	-6	52	16	10*	-12	26	40	4*
-19	39	57	-16*	0	14	38	-5*	-10	95	7	-2	-5	197	6	2	-11	44	22	-7*
-18	25	43	8*	1	40	12	14*	-9	69	8	5	-4	31	33	19*	-10	104	6	-3
-17	12	35	-5*	2	150	4	-2	-8	177	5	1	-3	166	5	5	-9	329	7	1
-16	77	8	8	3	94	7	1	-7	85	6	9	-2	0	37	-12*	-8	192	5	-5
-15	91	8	1	4	293	6	1	-6	239	6	1	-1	78	8	3	-7	426	13	-4
-14	111	6	-2	5	155	5	-6	-5	116	5	6	0	0	33	-17*	-6	274	6	10
-13	214	5	-5	6	333	8	-4	-4	233	5	-3	1	26	40	-10*	-5	499	16	-6
-12	239	6	-1	7	138	6	-7	-3	133	5	-8	2	8	43	-8*	-4	227	5	-23
-11	213	7	0	8	262	6	-6	-2	142	5	-7	3	121	6	3	-3	412	15	2
-10	254	6	-6	9	74	13	-4	-1	59	12	4*	4	47	14	3*	-2	45	28	-1*
-9	216	5	2	10	150	8	-4	0	59	22	12*	5	185	5	1	-1	285	9	16
-8	153	5	2	11	30	41	18*	1	56	13	-14*	6	54	12	3*	0	107	5	-3
-7	77	6	-2	12	24	34	-5*	2	126	5	-1	7	206	6	4	1	44	8	18
-6	29	30	2*	13	8	38	-20*	3	129	8	-1	8	57	12	6*	2	65	9	0
-5	83	5	7	14	90	11	-5	4	258	6	0	H,K=		5,	11	3	506	10	16
-4	212	5	5	15	50	16	-8*	5	95	6	7	-5	24	39	18*	4	168	4	-0
-3	204	5	-1	16	127	6	3	6	237	6	-6	-4	83	8	-2	5	505	13	8
-2	358	8	-0	H,K=		5,	7	7	80	9	-1	-3	41	17	12*	6	209	5	1
-1	255	6	0	-16	0	36	-1*	8	167	5	4	-2	148	7	-5	7	413	9	5
0	433	9	1	-15	132	6	18	9	54	16	1*	-1	44	15	12*	8	207	5	3
1	242	6	8	-14	0	40	-0*	10	84	9	3	0	178	5	-1	9	260	6	-2
2	287	6	-8	-13	197	6	2	11	0	35	-23*	1	30	41	-4*	10	48	26	-26*
3	263	6	3	-12	0	33	-4*	12	0	46	-2*	2	167	8	3	11	116	7	7
4	123	4	-4	-11	259	6	-3	13	42	18	22*	3	50	13	16*	12	23	39	13*
5	132	4	-2	-10	44	21	12*	H,K=		5,	9	4	115	6	15	13	77	26	4*
6	0	30	-9*	-9	206	5	1	-13	82	8	8	H,K=		6,	0	14	24	38	-25*
7	83	6	1	-8	44	36	42*	-12	153	6	3	-20	90	9	-17	15	131	11	-2
8	107	6	-4	-7	120	7	-3	-11	97	7	-2	-18	33	26	4*	16	61	17	-16*
9	137	6	-1	-6	49	21	18*	-10	164	6	-3	-16	96	8	5	17	173	6	-2
10	242	8	-1	-5	47	14	9*	-9	124	7	8	-14	272	6	1	18	79	12	-4
11	145	5	-5	-4	29	30	27*	-8	85	7	2	-12	336	7	-6	H,K=		6,	2
12	215	6	2	-3	250	7	0	-7	80	10	1	-10	336	7	-15	-20	76	11	-6

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-19	76	12	-1	-3	66	6	9	14	50	22	5*	-2	285	7	-2	-9	70	15	-8*
-18	51	18	32*	-2	356	10	-7	15	129	8	1	-1	176	5	3	-8	155	6	5
-17	11	49	5*	-1	96	4	13	16	28	41	5*	0	339	7	0	-7	1	32	-7*
-16	84	14	-3	0	0	27	-4*	17	0	40	-29*	1	133	4	6	-6	41	24	20*
-15	200	7	-2	1	47	14	-6*	H,K=		6,	5	2	271	6	2	-5	18	31	-9*
-14	173	6	-2	2	283	6	13	-18	134	8	-3	3	94	7	-0	-4	145	5	-1
-13	273	6	-8	3	44	9	9*	-17	109	7	-0	4	207	5	-8	-3	30	31	5*
-12	238	6	-3	4	409	9	-3	-16	144	11	-8	5	63	9	1	-2	265	6	2
-11	238	6	-10	5	83	5	-3	-15	101	7	-0	6	36	20	9*	-1	82	13	-14
-10	217	5	-7	6	442	14	-4	-14	125	6	-0	7	46	19	4*	0	263	6	-5
-9	252	6	-8	7	98	6	-6	-13	81	7	6	8	135	6	-5	1	152	5	1
-8	243	6	1	8	303	7	-0	-12	52	27	2*	9	81	12	-5	2	238	6	5
-7	176	4	4	9	26	34	-7*	-11	39	39	2*	10	205	6	-3	3	95	6	4
-6	0	27	-9*	10	174	5	4	-10	174	5	-7	11	119	6	-1	4	108	10	1
-5	90	4	-3	11	28	47	4*	-9	115	5	-3	12	213	6	4	5	39	15	16*
-4	203	5	-1	12	25	43	-1*	-8	272	6	-2	13	97	7	-5	6	43	13	34*
-3	281	6	-13	13	40	21	27*	-7	269	6	-3	14	149	6	-0	7	0	33	-4*
-2	423	10	9	14	96	10	7	-6	264	6	2	15	22	41	-30*	8	98	6	18
-1	368	11	-11	15	0	47	-28*	-5	218	5	1	H,K=		6,	7	9	52	14	-2*
0	413	11	-5	16	170	6	-4	-4	224	5	-1	-16	13	38	0*	10	151	6	-7
1	424	13	-14	17	35	46	-8*	-3	183	4	8	-15	166	7	3	11	71	10	-9
2	284	12	-4	18	168	9	7	-2	289	6	2	-14	0	37	-6*	12	184	7	4
3	345	7	-2	H,K=		6,	4	-1	137	4	-2	-13	66	10	-6	13	82	15	11
4	247	5	-0	-19	85	8	17	0	78	5	-1	-12	43	14	33*	H,K=		6,	9
5	93	5	-1	-18	34	46	10*	1	35	19	4*	-11	0	36	-26*	-12	0	40	-18*
6	89	6	6	-17	63	14	20*	2	176	4	4	-10	0	32	-2*	-11	46	15	15*
7	80	6	5	-16	44	23	17*	3	156	5	1	-9	168	6	0	-10	60	11	-8*
8	134	10	7	-15	125	7	-4	4	325	7	-9	-8	13	43	9*	-9	78	17	-2*
9	216	6	3	-14	109	6	2	5	230	6	-3	-7	298	7	-3	-8	152	5	-2
10	161	6	-6	-13	255	7	7	6	307	7	-3	-6	28	38	0*	-7	119	6	2
11	232	6	-1	-12	136	5	-2	7	197	5	-3	-5	354	7	5	-6	168	5	-3
12	218	6	-9	-11	337	7	-1	8	237	6	-2	-4	40	46	29*	-5	131	5	-2
13	202	6	-3	-10	0	34	-11*	9	141	9	-7	-3	282	6	-6	-4	187	5	-0
14	145	7	-6	-9	334	7	1	10	103	10	-3	-2	28	31	13*	-3	97	8	1
15	148	6	-5	-8	33	35	11*	11	71	9	-6	-1	141	6	3	-2	130	5	0
16	58	31	-0*	-7	173	5	9	12	13	34	11*	0	45	13	-12*	-1	19	32	-10*
17	56	57	5*	-6	83	5	-0	13	0	36	-14*	1	78	10	-2	0	26	33	2*
18	0	55	-13*	-5	162	4	7	14	92	8	7	2	23	41	-14*	1	34	40	12*
H,K=		6,	3	-4	31	14	25*	15	89	16	4	3	268	6	2	2	100	10	-1
-20	113	7	9	-3	308	7	4	16	114	10	-5	4	29	38	-2*	3	85	7	-7
-19	32	37	-7*	-2	144	4	-10	H,K=		6,	6	5	319	7	-4	4	137	7	-7
-18	182	6	2	-1	528	11	1	-17	46	33	20*	6	41	22	8*	5	113	6	-9
-17	61	12	-2*	0	121	4	3	-16	58	13	1*	7	273	6	1	6	138	10	-13
-16	204	5	0	1	531	11	-0	-15	65	12	-1*	8	10	32	10*	7	132	5	4
-15	58	17	1*	2	182	4	-0	-14	147	7	10	9	159	6	-3	8	141	6	-3
-14	204	5	2	3	320	7	-7	-13	70	11	8	10	29	33	12*	9	71	10	-10
-13	16	42	-6*	4	172	4	-4	-12	228	6	-8	11	44	17	-16*	10	75	10	-11
-12	36	34	-3*	5	125	4	5	-11	128	5	-5	12	42	28	39*	H,K=		6,	10
-11	62	19	7*	6	23	30	16*	-10	228	9	-6	13	41	29	8*	-9	153	6	-3
-10	160	6	-0	7	81	6	11	-9	126	12	-5	14	0	47	-9*	-8	14	37	-19*
-9	3	30	-34*	8	43	16	-23*	-8	186	6	-1	H,K=		6,	8	-7	55	13	1*
-8	341	7	1	9	236	6	-6	-7	69	8	-4	-14	103	7	-3	-6	0	36	-1*
-7	130	4	11	10	59	12	-6*	-6	48	11	11*	-13	88	11	15	-5	34	32	-8*
-6	489	12	0	11	318	7	-2	-5	0	42	-16*	-12	171	6	2	-4	42	15	11*
-5	31	13	5*	12	34	41	-19*	-4	120	8	-6	-11	125	7	8	-3	141	6	4
-4	529	11	2	13	225	6	-2	-3	112	5	-1	-10	223	6	-1	-2	46	17	-6*

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	203	5	-0	-3	347	10	-2	13	36	42	19*	-9	220	5	5	10	196	6	-1
0	53	12	4*	-2	328	7	1	14	38	47	-17*	-8	87	8	4	11	121	7	1
1	218	5	3	-1	434	11	-20	15	122	9	-10	-7	334	7	-1	12	177	8	-3
2	0	33	-21*	0	290	6	7	16	107	18	-10	-6	109	6	4	13	116	7	-9
3	140	6	-5	1	462	10	-5	17	151	7	2	-5	393	8	-10	14	99	9	-24
4	38	31	34*	2	228	5	2	18	100	14	-5	-4	110	5	7	15	87	10	8
5	63	11	-12	3	403	8	12	H,K=		7,	3	-3	394	8	1	16	47	24	3*
6	29	34	22*	4	261	6	9	-20	107	8	5	-2	37	11	28*	H,K=		7,	6
7	28	39	2*	5	180	5	4	-19	32	37	27*	-1	280	6	13	-17	68	12	-22
H,K=		6,	11	6	84	8	-9	-18	52	16	9*	0	0	31	-31*	-16	180	7	-1
-4	147	6	2	7	106	6	6	-17	13	37	-9*	1	75	5	10	-15	79	10	-11
-3	26	39	5*	8	98	7	3	-16	104	7	-11	2	25	28	7*	-14	134	7	2
-2	93	12	-3	9	241	7	-5	-15	20	49	-24*	3	322	7	-1	-13	26	33	13*
-1	13	37	10*	10	175	6	-8	-14	217	6	-9	4	25	38	-18*	-12	31	32	26*
0	17	35	-7*	11	287	7	-5	-13	52	15	-3*	5	391	8	-2	-11	60	11	23
1	25	34	18*	12	95	18	5*	-12	305	7	-1	6	72	9	21	-10	128	5	-2
2	44	18	-12*	13	210	6	-2	-11	83	7	1	7	320	7	-4	-9	85	11	-3
H,K=		7,	0	14	81	12	-11	-10	294	6	5	8	66	10	-13	-8	269	7	-0
-20	108	8	-8	15	134	7	8	-9	129	5	-9	9	216	7	0	-7	103	6	1
-18	192	6	-4	16	78	11	12	-8	273	6	3	10	49	14	5*	-6	369	8	-5
-16	250	6	-5	17	52	20	4*	-7	96	5	6	11	94	8	-10	-5	138	8	7
-14	231	7	-4	18	11	47	-10*	-6	56	7	2	12	27	39	25*	-4	275	7	2
-12	88	8	-11	H,K=		7,	2	-5	178	4	5	13	44	20	5*	-3	145	5	3
-10	177	5	4	-20	71	13	5	-4	192	5	2	14	44	19	24*	-2	176	5	-2
-8	421	9	-10	-19	127	8	1	-3	151	4	9	15	147	7	8	-1	65	10	3
-6	434	12	-17	-18	107	9	-6	-2	433	9	-1	16	17	42	2*	0	31	35	-7*
-4	537	11	-20	-17	155	6	7	-1	54	10	-6*	17	144	7	-8	1	38	26	-14*
-2	227	5	-13	-16	129	7	-14	0	510	14	5	H,K=		7,	5	2	160	5	-2
0	34	35	12*	-15	177	6	4	1	108	5	-20	-18	0	43	-7*	3	171	5	2
2	117	4	2	-14	102	11	1	2	398	12	7	-17	23	39	14*	4	259	6	-4
4	441	9	-1	-13	117	9	4	3	34	13	17*	-16	34	35	-18*	5	168	5	9
6	462	10	1	-12	27	37	19*	4	260	6	5	-15	77	9	-13	6	297	7	-3
8	343	8	-1	-11	56	16	22*	5	92	6	8	-14	105	6	6	7	53	16	-15*
10	167	6	-4	-10	112	6	-2	6	43	13	-14*	-13	183	5	-9	8	235	6	-5
12	29	61	21*	-9	276	6	9	7	0	33	-3*	-12	191	6	3	9	60	16	2*
14	102	14	-6	-8	222	5	-3	8	217	5	-2	-11	214	8	-3	10	137	7	5
16	167	10	3	-7	418	9	15	9	44	18	-2*	-10	288	6	0	11	34	40	21*
18	167	7	5	-6	329	7	-9	10	317	7	-1	-9	139	5	4	12	22	54	8*
H,K=		7,	1	-5	401	8	5	11	109	22	-7*	-8	213	6	-2	13	14	39	9*
-20	34	52	-0*	-4	282	6	-9	12	276	6	7	-7	69	8	-5	14	54	24	-17*
-19	62	16	-5*	-3	358	12	-18	13	63	16	-6*	-6	37	15	10*	15	24	40	-22*
-18	44	19	39*	-2	204	5	0	14	186	6	4	-5	45	11	-13*	H,K=		7,	7
-17	27	38	8*	-1	83	5	-18	15	44	23	17*	-4	149	4	6	-16	7	36	5*
-16	39	22	-1*	0	100	4	6	16	107	10	16	-3	153	6	-6	-15	111	9	4
-15	134	13	0	1	145	4	11	17	39	39	34*	-2	227	5	-0	-14	21	35	2*
-14	143	10	-14	2	243	5	1	H,K=		7,	4	-1	232	5	-1	-13	182	7	1
-13	290	7	-3	3	252	5	-2	-19	130	6	1	0	348	8	8	-12	0	34	-17*
-12	125	11	-12	4	279	6	1	-18	0	43	-23*	1	272	6	4	-11	221	5	3
-11	356	8	-16	5	360	8	-4	-17	182	6	-0	2	285	6	-5	-10	20	32	9*
-10	155	6	-3	6	311	7	-7	-16	25	35	7*	3	197	7	-6	-9	223	5	-5
-9	272	6	-7	7	350	7	4	-15	168	8	2	4	160	5	-10	-8	45	12	44*
-8	135	5	-4	8	159	6	1	-14	33	40	-6*	5	89	6	6	-7	121	8	3
-7	120	5	3	9	239	6	3	-13	147	11	-4	6	31	32	-11*	-6	68	11	18
-6	93	5	12	10	128	11	-1	-12	41	25	-3*	7	101	6	-9	-5	91	7	1
-5	34	14	27*	11	76	14	-7	-11	21	34	-22*	8	72	8	0	-4	49	37	6*
-4	102	6	-6	12	25	59	-18*	-10	24	36	2*	9	125	7	-3	-3	247	7	3

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	24	34	-16*	-1	132	5	7	-14	44	52	-39*	3	227	5	-3	-17	53	13	26*
-1	299	8	4	0	192	5	-2	-13	120	7	4	4	187	5	-7	-16	37	39	-2*
0	34	21	6*	1	100	7	-4	-12	35	37	23*	5	155	6	3	-15	120	7	-5
1	319	7	-3	2	173	5	0	-11	42	20	25*	6	49	13	4*	-14	87	8	12
2	52	18	28*	3	83	8	1	-10	80	11	-6	7	41	19	22*	-13	208	5	3
3	281	7	-10	4	91	7	18	-9	261	7	-6	8	110	6	8	-12	84	7	9
4	36	19	13*	5	45	14	1*	-8	258	7	-10	9	219	6	-11	-11	327	7	4
5	107	6	1	6	36	38	24*	-7	380	8	1	10	146	7	13	-10	24	37	2*
6	33	39	25*	7	41	18	28*	-6	321	7	4	11	210	9	-5	-9	307	7	5
7	50	12	-2*	8	64	10	13	-5	385	8	1	12	183	9	-1	-8	5	34	-2*
8	30	37	22*	9	77	11	5	-4	158	6	-15	13	147	6	-5	-7	144	5	3
9	147	6	-2	10	118	7	3	-3	393	8	-8	14	98	10	-14	-6	39	15	3*
10	36	38	29*	H,K=		7,	10	-2	33	20	-7*	15	130	7	7	-5	84	6	-7
11	201	6	-6	-9	100	12	1	-1	250	5	2	16	40	40	-10*	-4	56	8	-1
12	17	40	-1*	-8	44	19	14*	0	77	6	-4	17	63	14	9*	-3	293	6	0
13	195	6	-2	-7	164	6	1	1	144	4	2	H,K=		8,	3	-2	109	5	7
H,K=		7,	8	-6	44	29	22*	2	36	14	25*	-19	0	41	-39*	-1	408	9	12
-14	90	8	3	-5	202	5	10	3	317	7	9	-18	160	7	1	0	138	6	-0
-13	54	12	12*	-4	38	21	3*	4	72	13	-19	-17	56	15	4*	1	423	9	2
-12	28	37	13*	-3	166	6	-7	5	356	8	-5	-16	204	7	9	2	103	5	5
-11	33	33	21*	-2	48	15	9*	6	191	5	1	-15	64	13	-6*	3	298	7	-1
-10	66	9	14	-1	67	9	-6	7	338	7	3	-14	194	5	10	4	34	24	27*
-9	78	8	2	0	31	38	22*	8	200	6	-1	-13	30	35	18*	5	133	5	-10
-8	148	6	-3	1	33	33	5*	9	266	8	-12	-12	97	10	-11	6	44	14	15*
-7	92	11	-3	2	44	16	14*	10	93	15	1	-11	34	48	-13*	7	59	11	-9*
-6	212	5	6	3	117	7	-0	11	97	10	10	-10	96	11	3	8	39	23	23*
-5	109	8	8	4	17	35	-5*	12	0	43	-12*	-9	17	41	-15*	9	228	6	-8
-4	232	5	-3	5	176	6	6	13	52	16	-3*	-8	309	7	1	10	53	15	6*
-3	70	8	-4	6	31	35	-3*	14	30	38	-2*	-7	87	6	3	11	221	6	-3
-2	177	5	0	H,K=		8,	0	15	128	7	-1	-6	488	10	-0	12	46	17	6*
-1	40	16	-2*	-20	80	10	-2	16	75	11	8	-5	148	4	-3	13	194	7	1
0	51	11	8*	-18	53	16	22*	17	143	8	-13	-4	458	10	-3	14	43	26	19*
1	44	13	11*	-16	75	18	6*	H,K=		8,	2	-3	68	7	8	15	108	8	0
2	122	6	-5	-14	202	7	-2	-20	79	14	2	-2	261	6	-4	16	62	13	34*
3	77	8	-7	-12	282	7	-6	-19	66	14	5*	-1	55	8	-12	H,K=		8,	5
4	224	5	-0	-10	324	7	4	-18	39	39	30*	0	0	29	-13*	-18	130	6	3
5	75	8	-9	-8	232	7	7	-17	66	16	53*	1	51	10	18*	-17	99	7	-6
6	193	6	-0	-6	144	6	2	-16	66	13	-15*	2	192	6	-3	-16	137	6	-1
7	70	11	9	-4	141	6	-19	-15	125	7	-5	3	114	5	9	-15	106	8	6
8	162	5	-3	-2	427	9	-10	-14	171	8	-0	4	301	7	-4	-14	111	9	2
9	74	9	9	0	548	11	6	-13	242	8	-7	5	74	8	-6	-13	40	22	-12*
10	99	7	7	2	515	11	4	-12	237	7	4	6	354	8	-4	-12	28	41	24*
11	29	44	-3*	4	381	8	3	-11	285	7	-0	7	103	7	-0	-11	45	14	13*
12	0	41	-6*	6	71	9	-8	-10	206	5	-5	8	333	7	-3	-10	136	5	-10
H,K=		7,	9	8	224	6	1	-9	260	7	-5	9	11	47	-10*	-9	140	5	2
-12	118	6	3	10	347	8	-1	-8	171	6	-1	10	171	6	0	-8	201	6	-10
-11	109	7	-4	12	268	7	3	-7	125	5	2	11	10	40	-23*	-7	230	5	2
-10	150	6	1	14	163	6	5	-6	39	13	-6*	12	47	17	18*	-6	233	5	1
-9	121	8	2	16	102	14	4	-5	38	15	3*	13	39	27	28*	-5	211	5	-4
-8	93	10	3	H,K=		8,	1	-4	193	5	7	14	108	8	-9	-4	275	6	-2
-7	72	8	10	-20	58	29	-4*	-3	225	5	0	15	11	40	-14*	-3	130	5	-11
-6	18	33	1*	-19	125	7	-2	-2	224	5	-4	16	152	7	3	-2	174	5	-3
-5	0	34	-18*	-18	96	8	-6	-1	492	16	-2	17	45	49	-7*	-1	94	7	3
-4	62	10	-9	-17	177	7	-9	0	258	6	-1	H,K=		8,	4	0	16	30	-7*
-3	114	10	1	-16	106	7	-3	1	337	7	-18	-19	72	18	10*	1	36	17	31*
-2	131	8	-3	-15	181	6	-6	2	324	7	-1	-18	23	43	17*	2	144	6	-2

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	166	5	-2	-6	43	19	24*	-3	110	6	5	-12	129	11	-5	6	190	5	1
4	277	6	-1	-5	324	7	1	-2	113	7	4	-11	305	7	-9	7	295	6	-4
5	186	5	-11	-4	57	9	26	-1	44	18	11*	-10	149	6	-2	8	191	5	-6
6	246	6	5	-3	261	6	7	0	0	34	-9*	-9	259	6	-6	9	237	7	3
7	228	6	-4	-2	66	9	-11	1	50	18	14*	-8	129	5	-5	10	110	9	1
8	165	5	11	-1	145	7	-3	2	73	8	7	-7	188	5	0	11	90	6	12
9	127	6	-13	0	16	46	7*	3	98	6	-3	-6	20	31	-8*	12	5	40	-9*
10	95	7	-7	1	53	13	23*	4	145	6	2	-5	39	12	1*	13	63	10	-6
11	79	8	7	2	20	35	-14*	5	128	5	9	-4	64	9	-3	14	70	10	-7
12	45	17	11*	3	199	6	-5	6	145	7	-9	-3	259	6	-6	15	123	7	2
13	51	16	15*	4	54	18	5*	7	106	6	3	-2	136	4	7	16	82	9	-15
14	40	41	-28*	5	278	6	-2	8	119	9	-1	-1	531	11	4	H,K=		9,	3
15	78	10	0	6	42	18	22*	9	56	15	-11*	0	254	5	6	-19	27	44	7*
H,K=		8,	6	7	208	6	-1	H,K=		8,	10	1	507	10	9	-18	0	44	-14*
-17	33	47	12*	8	40	23	31*	-8	24	35	20*	2	159	4	1	-17	37	40	6*
-16	42	21	-5*	9	146	6	-4	-7	71	13	12	3	291	7	-3	-16	96	10	-3
-15	63	11	5	10	30	34	21*	-6	21	35	1*	4	122	5	-2	-15	40	23	9*
-14	150	6	8	11	77	9	3	-5	53	13	7*	5	96	5	12	-14	191	6	-1
-13	63	11	-18	12	39	23	25*	-4	41	16	22*	6	12	31	6*	-13	37	44	-7*
-12	202	5	1	13	45	22	23*	-3	124	8	-1	7	72	8	-1	-12	261	7	-5
-11	89	12	3	H,K=		8,	8	-2	51	15	11*	8	89	10	10	-11	52	15	-8*
-10	211	7	5	-14	95	8	-10	-1	187	7	3	9	154	7	0	-10	284	7	4
-9	107	7	-2	-13	64	10	17	0	60	11	5	10	133	6	5	-9	44	15	-7*
-8	197	6	1	-12	172	5	1	1	201	5	12	11	241	6	-4	-8	197	6	2
-7	41	16	0*	-11	92	12	13	2	7	35	-17*	12	83	7	-5	-7	19	49	-3*
-6	78	12	3	-10	194	5	4	3	146	5	3	13	176	6	-6	-6	0	36	-25*
-5	67	9	13	-9	71	13	-4*	4	34	43	31*	14	62	11	5	-5	95	6	0
-4	170	6	1	-8	139	5	3	5	36	37	-20*	15	126	6	-1	-4	144	5	-1
-3	88	6	-1	-7	40	16	19*	H,K=		9,	0	16	77	11	23	-3	106	5	1
-2	264	6	3	-6	4	32	-15*	-20	125	7	9	17	54	15	2*	-2	386	8	4
-1	116	6	12	-5	24	35	15*	-18	191	5	-2	H,K=		9,	2	-1	30	30	5*
0	312	7	-4	-4	90	9	-4	-16	235	6	-15	-19	95	16	-16	0	434	13	-7
1	113	6	-8	-3	61	9	4	-14	161	5	-3	-18	95	9	-6	1	33	18	18*
2	315	7	-11	-2	192	6	7	-12	79	9	11	-17	149	7	-1	2	338	7	-15
3	141	5	-2	-1	109	5	3	-10	84	7	-4	-16	118	8	-17	3	81	7	8
4	207	7	0	0	205	7	-2	-8	369	8	-5	-15	156	7	-9	4	192	7	-9
5	25	33	-10*	1	116	5	2	-6	460	10	-11	-14	101	8	-5	5	77	10	2
6	0	37	-15*	2	203	5	2	-4	379	8	-3	-13	77	27	-3*	6	89	8	-5
7	0	32	-24*	3	69	8	10	-2	279	6	-13	-12	26	38	7*	7	72	9	32
8	146	6	0	4	137	5	3	0	101	6	-4	-11	63	13	-4*	8	150	6	0
9	73	10	1	5	0	35	-14*	2	213	5	-5	-10	83	9	-7	9	120	9	5
10	179	5	6	6	0	37	-9*	4	343	7	-6	-9	174	7	-7	10	254	7	-3
11	107	13	1	7	39	18	23*	6	352	8	-9	-8	192	5	0	11	26	37	-2*
12	170	7	-5	8	63	11	-6	8	295	7	-10	-7	321	7	-0	12	221	8	-2
13	100	8	5	9	35	40	-3*	10	261	12	-7	-6	343	8	3	13	19	39	-14*
14	128	17	-5	10	129	7	-7	12	12	40	-5*	-5	348	8	2	14	164	6	-1
H,K=		8,	7	11	65	11	-7	14	104	8	-1	-4	299	7	-2	15	63	13	24*
-15	156	7	-3	H,K=		8,	9	16	147	8	2	-3	191	5	-5	16	79	12	-11
-14	0	40	-4*	-11	0	53	-12*	H,K=		9,	1	-2	194	5	-1	H,K=		9,	4
-13	83	13	5	-10	74	9	13	-19	58	12	6*	-1	63	7	3	-18	51	16	19*
-12	22	34	9*	-9	63	10	-3	-18	0	36	-20*	0	0	29	-15*	-17	170	7	2
-11	16	34	-13*	-8	130	8	-2	-17	39	24	32*	1	71	8	13	-16	20	44	-23*
-10	28	32	20*	-7	102	10	-4	-16	32	35	16*	2	177	5	3	-15	181	6	3
-9	138	5	2	-6	166	5	1	-15	126	8	-4	3	158	5	6	-14	32	46	10*
-8	42	15	12*	-5	125	8	5	-14	88	7	-1	4	241	5	-1	-13	140	5	4
-7	272	6	8	-4	160	6	-4	-13	250	7	-3	5	293	6	7	-12	50	17	22*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-11	34	46	11*	11	97	12	-13	5	101	6	-1	-3	149	6	6	10	81	25	1*
-10	29	52	24*	12	135	10	-1	6	43	19	25*	-2	14	34	-17*	11	97	8	0
-9	206	6	-2	13	119	10	-5	7	57	34	-2*	-1	85	7	11	12	15	38	8*
-8	93	6	11	14	106	8	-6	8	41	17	38*	0	41	18	37*	13	32	40	-20*
-7	311	7	-5	H,K=	9,	6		9	118	6	-8	1	46	21	29*	14	30	39	-13*
-6	131	5	-5	-16	149	6	-3	10	12	35	10*	2	19	38	-2*	15	122	7	-2
-5	376	8	5	-15	74	9	1	11	172	6	-4	3	98	7	-1	16	32	41	-27*
-4	129	5	-9	-14	98	8	-14	12	35	40	28*	H,K=	10,	0		H,K=	10,	2	
-3	357	8	1	-13	44	17	4*	H,K=	9,	8		-18	38	39	7*	-19	70	12	33
-2	110	7	1	-12	37	38	31*	-13	18	46	-11*	-16	22	47	-2*	-18	0	40	-6*
-1	160	5	2	-11	44	15	18*	-12	5	37	-33*	-14	167	5	4	-17	0	40	-7*
0	26	30	9*	-10	99	6	-6	-11	0	34	-20*	-12	272	7	-4	-16	79	15	-2*
1	31	24	14*	-9	76	15	-17*	-10	77	9	13	-10	365	8	-6	-15	79	11	-8
2	75	10	0	-8	204	5	-0	-9	70	9	-6	-8	292	7	0	-14	111	8	-11
3	220	5	-1	-7	114	6	-5	-8	147	5	1	-6	84	9	-9	-13	218	7	-9
4	54	23	3*	-6	260	7	-3	-7	84	7	-0	-4	121	5	5	-12	154	9	-2
5	317	7	-5	-5	138	8	2	-6	196	5	2	-2	369	8	-8	-11	265	6	-4
6	45	17	9*	-4	238	6	2	-5	88	8	-3	0	576	12	-6	-10	157	6	2
7	338	7	-6	-3	134	5	-2	-4	218	5	1	2	451	9	-8	-9	198	6	6
8	110	9	7	-2	135	5	4	-3	77	8	-8	4	164	6	-10	-8	159	5	-1
9	194	6	-4	-1	40	16	1*	-2	164	5	-2	6	27	35	-7*	-7	74	12	0
10	44	18	-7*	0	51	13	17*	-1	36	20	-4*	8	79	8	6	-6	41	17	-1*
11	79	12	-9	1	98	6	17	0	43	14	24*	10	191	6	-1	-5	37	20	-2*
12	45	32	29*	2	117	5	-2	1	31	32	13*	12	258	6	-5	-4	152	7	2
13	50	17	12*	3	122	6	-0	2	100	6	4	14	163	5	-2	-3	223	5	-3
14	33	39	-1*	4	201	5	-1	3	64	11	15	16	75	20	-17*	-2	204	5	5
15	124	8	-4	5	116	6	-5	4	167	7	-7	H,K=	10,	1	-1	355	8	-1	
H,K=	9,	5		6	248	6	-6	5	104	10	6	-19	125	10	2	0	217	5	-2
-17	23	36	14*	7	73	10	0	6	207	6	-2	-18	85	10	-1	1	372	8	-13
-16	53	20	3*	8	205	6	2	7	87	14	-9	-17	165	9	-14	2	179	5	3
-15	69	10	0	9	45	54	-14*	8	144	6	2	-16	84	10	-8	3	222	6	-0
-14	87	11	-10	10	69	18	-21*	9	40	31	-23*	-15	184	6	-4	4	100	8	-3
-13	152	5	1	11	44	24	1*	10	69	14	-3*	-14	65	12	-3*	5	74	9	8
-12	176	5	0	12	0	39	-18*	H,K=	9,	9		-13	105	8	12	6	41	44	2*
-11	158	6	2	13	40	61	36*	-10	125	12	-4	-12	58	34	8*	7	71	11	-9
-10	262	6	-1	H,K=	9,	7		-9	86	10	-6	-11	0	39	-30*	8	26	43	-3*
-9	127	8	-6	-15	101	11	8	-8	81	8	1	-10	125	6	3	9	118	15	-2
-8	212	6	-0	-14	25	35	-4*	-7	27	41	-0*	-9	173	7	-4	10	168	6	4
-7	95	8	-3	-13	160	6	2	-6	35	23	31*	-8	177	5	4	11	183	6	6
-6	43	15	-15*	-12	0	34	-11*	-5	51	12	14*	-7	292	6	1	12	138	6	3
-5	35	20	-6*	-11	191	6	-1	-4	84	7	6	-6	163	5	-3	13	171	9	-1
-4	106	6	7	-10	26	36	2*	-3	55	11	-9*	-5	375	8	2	14	88	10	-22
-3	175	5	-10	-9	200	5	-3	-2	134	6	-7	-4	146	5	-2	15	119	7	12
-2	230	6	-3	-8	32	41	9*	-1	97	7	3	-3	357	8	4	H,K=	10,	3	
-1	224	5	-4	-7	133	5	-2	0	155	5	-3	-2	44	22	-10*	-18	159	7	7
0	267	6	0	-6	50	11	12*	1	114	6	-6	-1	172	5	-3	-17	32	46	-21*
1	237	5	-6	-5	33	36	-10*	2	123	6	-5	0	72	9	1	-16	200	8	3
2	289	6	-6	-4	30	38	-7*	3	124	8	7	1	79	7	8	-15	38	38	-6*
3	130	8	-7	-3	200	5	-5	4	102	11	-4	2	40	17	-0*	-14	182	6	5
4	190	5	-3	-2	17	38	13*	5	19	41	-20*	3	218	5	10	-13	8	40	-22*
5	37	40	21*	-1	250	6	-2	6	28	35	7*	4	122	6	-9	-12	84	12	28
6	41	21	24*	0	25	36	11*	7	0	36	-27*	5	305	7	4	-11	55	20	-3*
7	48	25	23*	1	275	6	-6	H,K=	9,	10		6	199	6	-7	-10	107	8	-6
8	129	6	-4	2	23	32	15*	-6	34	35	10*	7	278	6	2	-9	94	8	14
9	73	9	-6	3	225	5	-4	-5	168	6	3	8	102	15	-2	-8	230	6	-3
10	133	6	-7	4	14	40	8*	-4	18	38	-13*	9	243	8	7	-7	97	6	10

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	383	8	7	H,K=	10,		5	7	26	34	-1*	H,K=	10,		9	-3	235	6	5
-5	89	7	-5	-17	110	10	4	8	89	8	-8	-9	75	9	2	-2	128	6	-3
-4	395	8	-3	-16	138	9	-2	9	66	11	-5	-8	117	6	6	-1	336	7	-7
-3	44	14	-6*	-15	95	7	12	10	156	5	4	-7	119	6	8	0	163	7	-7
-2	259	6	8	-14	111	7	5	11	74	11	-14	-6	140	7	1	1	345	7	-2
-1	29	38	21*	-13	38	50	2*	12	154	6	4	-5	104	6	-2	2	167	5	-2
0	34	26	5*	-12	14	45	-2*	H,K=	10,		7	-4	136	7	0	3	248	6	-9
1	43	21	8*	-11	20	35	-20*	-14	33	40	23*	-3	101	14	4	4	67	10	13
2	137	5	2	-10	102	6	-3	-13	70	15	7*	-2	87	7	-5	5	96	10	5
3	37	46	-15*	-9	106	7	3	-12	13	42	11*	-1	73	12	10	6	29	37	-9*
4	312	7	-7	-8	189	5	-8	-11	0	45	-20*	0	32	43	16*	7	24	48	-2*
5	107	9	-4	-7	175	8	-5	-10	19	37	15*	1	27	48	8*	8	89	14	-5
6	357	8	-3	-6	192	5	7	-9	129	8	1	2	55	27	-6*	9	120	6	-4
7	112	8	-1	-5	194	5	2	-8	41	16	37*	3	71	11	-9	10	42	39	9*
8	293	7	5	-4	210	5	7	-7	231	6	6	4	112	7	-5	11	201	6	-0
9	40	52	8*	-3	137	5	-1	-6	14	33	2*	5	119	7	6	12	73	17	-5*
10	123	6	1	-2	181	5	-3	-5	258	6	-2	6	136	6	2	13	199	6	5
11	58	13	32*	-1	91	9	2	-4	46	20	33*	H,K=	10,		10	14	78	11	6
12	26	39	23*	0	87	7	4	-3	223	5	-1	-3	100	7	-3	15	107	13	-1
13	27	39	5*	1	20	34	-13*	-2	34	42	23*	-2	20	37	-14*	H,K=	11,		2
14	96	9	-0	2	88	11	-0	-1	120	6	-2	-1	151	8	4	-18	102	12	-8
15	0	41	-27*	3	175	8	3	0	25	36	-8*	0	41	21	-5*	-17	138	7	-1
H,K=	10,		4	4	186	6	-1	1	36	20	-9*	H,K=	11,		0	-16	135	11	-5
-18	26	39	22*	5	161	9	-2	2	25	33	-16*	-18	175	10	4	-15	140	6	1
-17	32	41	13*	6	204	5	2	3	152	7	-3	-16	174	6	-1	-14	86	10	-6
-16	7	37	1*	7	155	5	5	4	30	33	27*	-14	141	6	2	-13	62	12	-2*
-15	102	12	2	8	165	5	-2	5	201	6	-3	-12	37	56	4*	-12	57	37	16*
-14	32	36	-14*	9	146	6	2	6	38	41	30*	-10	95	13	5	-11	41	41	-27*
-13	183	6	6	10	94	12	3	7	223	6	0	-8	295	7	-4	-10	68	11	-12
-12	49	23	-10*	11	77	9	30	8	15	35	11*	-6	292	6	-9	-9	128	7	-2
-11	289	7	-4	12	21	45	-2*	9	142	6	-2	-4	338	7	5	-8	168	6	-1
-10	32	40	1*	13	44	29	16*	10	0	37	-8*	-2	323	8	2	-7	197	6	1
-9	280	7	-11	H,K=	10,		6	11	56	14	12*	0	61	13	-4*	-6	272	7	-7
-8	0	34	-8*	-16	41	23	-9*	H,K=	10,		8	2	174	7	1	-5	265	6	-0
-7	151	7	-2	-15	8	37	-49*	-12	125	8	-4	4	298	8	3	-4	249	7	3
-6	43	17	-4*	-14	119	6	1	-11	80	12	5	6	332	7	-8	-3	265	6	-6
-5	13	42	-11*	-13	53	20	3*	-10	156	6	-2	8	270	8	-12	-2	164	5	2
-4	34	24	5*	-12	186	6	0	-9	73	13	-0	10	158	6	-7	-1	145	5	4
-3	187	5	-7	-11	47	16	-7*	-8	136	5	5	12	47	19	17*	0	15	36	11*
-2	58	12	-1*	-10	200	6	2	-7	33	39	7*	14	72	12	-16	1	10	38	-3*
-1	349	8	6	-9	112	6	8	-6	59	10	15	H,K=	11,		1	2	118	7	4
0	76	7	13	-8	184	5	-2	-5	38	18	37*	-18	41	54	29*	3	198	10	0
1	339	8	-8	-7	51	11	3*	-4	83	12	2	-17	14	45	13*	4	164	10	-9
2	51	18	38*	-6	48	22	2*	-3	77	7	19	-16	28	47	22*	5	260	6	-7
3	295	6	2	-5	38	43	-0*	-2	152	6	-0	-15	78	11	4	6	172	6	-0
4	17	34	11*	-4	163	5	-8	-1	109	9	1	-14	27	39	-37*	7	227	7	-0
5	124	7	6	-3	108	10	-14	0	177	5	4	-13	205	6	-3	8	174	6	1
6	46	51	24*	-2	273	6	-6	1	89	7	6	-12	156	8	-13	9	124	6	1
7	59	11	21*	-1	112	5	4	2	159	5	-8	-11	288	9	-13	10	77	9	13
8	0	36	-39*	0	292	6	4	3	49	15	2*	-10	138	13	-10	11	79	12	-2
9	168	7	-4	1	89	7	-2	4	142	6	-7	-9	287	7	-11	12	41	28	22*
10	49	18	31*	2	250	6	-2	5	61	13	18*	-8	56	16	-6*	13	39	40	13*
11	167	6	1	3	63	12	-6*	6	40	20	10*	-7	126	8	1	14	37	54	-2*
12	63	14	-2*	4	141	6	2	7	0	45	-2*	-6	21	35	8*	15	71	14	-10*
13	176	7	4	5	79	7	14	8	60	15	-21*	-5	84	9	4	H,K=	11,		3
14	20	44	-23*	6	36	22	13*	9	41	41	-3*	-4	17	40	8*	-18	59	43	46*

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-17	49	55	37*	6	81	8	-3	2	86	7	8	-8	91	7	17	6	114	8	1
-16	79	13	10	7	231	6	2	3	94	6	7	-7	24	35	4*	7	248	6	-7
-15	48	20	4*	8	47	25	7*	4	169	5	-3	-6	26	36	17*	8	65	14	-13*
-14	146	6	2	9	165	6	-1	5	54	29	-22*	-5	0	35	-21*	9	177	6	1
-13	62	18	24*	10	49	16	26*	6	194	6	-7	-4	68	12	11	10	41	22	-2*
-12	249	6	3	11	61	14	-3*	7	81	12	-17	-3	54	34	-1*	11	46	55	-24*
-11	34	42	-8*	12	15	39	9*	8	173	6	-4	-2	121	7	3	12	30	38	1*
-10	278	6	-1	13	0	42	-28*	9	70	11	-4	-1	112	7	10	13	42	55	20*
-9	0	51	-20*	H,K=	11,	5		10	95	18	2*	0	137	5	5	14	21	49	-10*
-8	157	6	4	-16	26	37	-6*	11	31	40	-0*	1	107	7	-6	H,K=	12,	2	
-7	79	8	0	-15	45	30	-9*	H,K=	11,	7		2	112	8	-4	-17	7	40	-6*
-6	52	14	-3*	-14	104	7	10	-13	139	6	-2	3	84	9	-6	-16	50	17	12*
-5	46	15	-1*	-13	125	6	9	-12	20	35	10*	4	73	12	-8	-15	71	11	9
-4	122	7	3	-12	153	6	6	-11	168	6	-2	H,K=	12,	0	-14	78	10	-7	
-3	112	6	-9	-11	180	7	1	-10	23	39	12*	-18	49	21	7*	-13	153	6	-7
-2	267	7	-1	-10	214	5	7	-9	211	6	9	-16	47	26	12*	-12	131	8	7
-1	19	35	-21*	-9	131	9	5	-8	34	34	21*	-14	146	7	2	-11	238	6	3
0	339	7	-2	-8	183	5	3	-7	147	5	5	-12	318	7	4	-10	170	6	-1
1	0	34	-12*	-7	29	38	-7*	-6	32	34	19*	-10	362	8	-9	-9	177	6	-5
2	318	7	-1	-6	36	23	-3*	-5	47	21	16*	-8	263	9	1	-8	84	9	0
3	60	12	-23*	-5	75	13	-3	-4	48	13	11*	-6	67	12	-14	-7	56	13	15*
4	259	6	-0	-4	100	6	-8	-3	169	5	-2	-4	96	7	-11	-6	47	16	41*
5	23	50	-20*	-3	114	7	-3	-2	0	32	-11*	-2	217	5	-5	-5	63	12	-2*
6	57	16	-3*	-2	223	8	-3	-1	211	6	6	0	386	8	-5	-4	112	6	-2
7	38	23	27*	-1	181	5	2	0	10	36	-13*	2	400	8	-5	-3	134	6	-0
8	106	8	-3	0	251	7	2	1	217	6	9	4	228	6	-4	-2	119	6	3
9	63	11	-2	1	206	6	-5	2	14	37	-3*	6	40	35	-19*	-1	257	6	3
10	170	7	-1	2	203	5	7	3	170	6	-2	8	101	7	-9	0	124	9	-3
11	0	46	-37*	3	105	6	-8	4	6	38	-5*	10	169	6	-13	1	270	6	-0
12	186	7	2	4	92	11	-7	5	105	10	-5	12	187	6	3	2	156	6	1
13	36	39	13*	5	35	40	15*	6	13	35	-13*	14	143	7	1	3	185	6	-5
14	178	6	10	6	0	37	-16*	7	20	54	14*	H,K=	12,	1	4	154	8	8	
H,K=	11,	4	7	0	35	-8*	8	31	39	31*	-18	59	18	-20*	5	67	27	-3*	
-17	171	6	2	8	88	8	1	9	114	7	-12	-17	159	8	-0	6	64	11	15
-16	63	15	39*	9	48	20	-11*	10	35	43	25*	-16	60	15	6*	7	58	12	-3*
-15	170	6	5	10	132	7	-4	H,K=	11,	8		-15	145	7	7	8	68	18	-4*
-14	44	20	14*	11	125	9	5	-11	12	46	-6*	-14	46	22	2*	9	113	8	-1
-13	87	8	4	12	147	6	14	-10	39	28	-4*	-13	89	8	6	10	138	9	-11
-12	38	24	-2*	H,K=	11,	6		-9	39	46	-2*	-12	14	42	2*	11	114	10	-8
-11	42	24	3*	-15	62	14	-7*	-8	137	6	5	-11	0	36	-9*	12	110	8	-2
-10	0	37	-5*	-14	80	9	-4	-7	81	10	10	-10	31	53	-2*	13	125	12	-9
-9	168	6	9	-13	32	36	7*	-6	187	5	3	-9	130	12	-4	14	67	14	-15*
-8	62	19	-11*	-12	22	36	14*	-5	84	8	3	-8	65	11	15	H,K=	12,	3	
-7	221	7	3	-11	0	54	-20*	-4	191	9	1	-7	280	6	-7	-17	38	40	-9*
-6	141	6	2	-10	85	8	-2	-3	82	8	-1	-6	127	6	5	-16	157	12	-3
-5	315	7	10	-9	62	10	2	-2	137	6	3	-5	296	7	-4	-15	63	13	13*
-4	132	7	1	-8	143	5	-1	-1	27	34	-10*	-4	120	7	-8	-14	131	6	14
-3	299	7	2	-7	120	6	-4	0	39	18	12*	-3	296	7	-4	-13	0	40	-6*
-2	0	34	-23*	-6	218	7	1	1	0	46	-7*	-2	110	6	-2	-12	58	30	11*
-1	202	5	-6	-5	131	6	4	2	68	13	-9*	-1	169	5	7	-11	63	11	23
0	7	34	-34*	-4	223	5	9	3	62	10	3	0	43	48	28*	-10	52	16	-5*
1	26	42	7*	-3	97	6	2	4	140	6	-3	1	52	33	8*	-9	41	25	2*
2	0	36	-21*	-2	131	5	-7	5	90	10	7	2	43	19	-9*	-8	204	8	1
3	234	6	-2	-1	9	50	-3*	6	176	6	5	3	185	5	-1	-7	38	44	30*
4	45	23	-4*	0	0	44	-41*	7	76	10	-0	4	107	11	-8	-6	350	8	0
5	306	7	3	1	61	11	18	H,K=	11,	9		5	247	6	-1	-5	83	9	-9

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	369	8	-3	-8	120	8	1	-3	188	7	-2	-16	31	39	-11*	8	104	9	-5
-3	33	36	-4*	-7	111	8	-10	-2	40	19	15*	-15	94	16	8	9	146	6	13
-2	185	5	1	-6	169	6	-5	-1	67	17	-18*	-14	70	12	-0	10	65	18	15*
-1	0	38	-4*	-5	144	6	-0	0	52	13	21*	-13	182	6	3	11	79	10	16
0	0	37	-23*	-4	236	6	2	1	22	38	-7*	-12	127	6	8	12	11	49	3*
1	9	45	2*	-3	132	7	0	2	5	43	-11*	-11	241	6	1	H,K=	13,	3	
2	152	8	0	-2	187	5	0	3	125	6	5	-10	96	12	7	-16	35	54	-14*
3	84	12	12	-1	56	15	-26*	4	0	44	-19*	-9	230	8	-0	-15	17	38	-7*
4	277	7	7	0	35	26	-12*	5	173	8	-4	-8	72	17	-2*	-14	116	8	-16
5	57	15	-20*	1	39	22	-2*	6	22	38	5*	-7	102	7	10	-13	69	16	18*
6	293	8	9	2	80	8	-13	7	187	6	2	-6	31	39	11*	-12	192	6	-2
7	33	36	13*	3	93	15	2	8	0	39	-4*	-5	90	10	9	-11	0	38	-42*
8	178	7	7	4	149	5	-5	H,K=	12,	8	-4	94	8	-12	-10	251	6	3	
9	28	38	6*	5	125	6	4	-10	112	7	2	-3	103	9	-2	-9	55	26	27*
10	100	9	2	6	154	6	-1	-9	48	17	-11*	-2	93	9	-5	-8	179	10	3
11	0	40	-12*	7	139	6	4	-8	102	12	-10	-1	203	10	-6	-7	0	38	-4*
12	0	41	-20*	8	154	6	7	-7	41	30	2*	0	120	7	-2	-6	69	10	37
13	32	43	31*	9	105	9	-0	-6	56	11	15*	1	309	7	-8	-5	26	46	6*
H,K=	12,	4	10	114	7	-1	-5	0	42	-8*	2	103	10	-2	-4	102	17	-3	
-16	0	47	-18*	11	40	30	18*	-4	54	13	-1*	3	247	7	-19	-3	84	12	-3
-15	91	8	3	H,K=	12,	6	-3	78	8	5	4	47	49	-5*	-2	170	6	3	
-14	40	46	11*	-14	113	11	-1	-2	136	6	0	5	72	10	-25	-1	47	52	-26*
-13	177	7	0	-13	75	19	8*	-1	105	8	-1	6	47	20	20*	0	230	10	-7
-12	30	40	-4*	-12	167	7	-1	0	172	9	4	7	51	14	7*	1	48	19	-11*
-11	265	7	3	-11	73	11	3	1	84	8	6	8	24	37	-28*	2	313	9	-3
-10	86	8	12	-10	183	7	8	2	163	5	-2	9	148	9	3	3	37	30	-0*
-9	241	7	3	-9	77	11	-5	3	42	25	-21*	10	27	50	-23*	4	223	6	-10
-8	46	15	13*	-8	136	6	8	4	115	13	1	11	149	7	-5	5	21	44	13*
-7	116	11	-7	-7	65	15	16*	5	47	22	17*	12	45	24	-14*	6	45	18	5*
-6	26	39	-26*	-6	37	48	-0*	6	42	20	22*	13	128	14	1	7	34	36	26*
-5	0	50	-5*	-5	51	14	-4*	H,K=	12,	9	H,K=	13,	2	8	109	10	17		
-4	54	27	16*	-4	122	6	0	-5	107	7	0	-17	128	7	8	9	0	38	-24*
-3	179	5	-0	-3	102	6	-2	-4	119	10	2	-16	90	10	-10	10	138	7	-3
-2	54	12	6*	-2	187	6	4	-3	116	6	8	-15	82	11	-9	11	42	26	8*
-1	282	7	5	-1	86	7	-6	-2	76	9	-1	-14	86	10	-5	12	155	7	-1
0	45	17	30*	0	198	5	4	-1	63	15	8*	-13	63	15	8*	H,K=	13,	4	
1	321	8	5	1	64	12	-3*	0	0	38	-9*	-12	57	13	17*	-15	143	10	-3
2	98	10	11	2	192	5	-6	1	43	19	11*	-11	27	37	13*	-14	41	24	9*
3	238	7	8	3	78	8	4	H,K=	13,	0	-10	44	19	-5*	-13	54	16	-13*	
4	92	14	16	4	127	6	2	-16	149	11	10	-9	63	12	-7*	-12	36	43	-9*
5	101	7	-8	5	53	14	-3*	-14	113	8	9	-8	154	6	-11	-11	31	36	28*
6	51	13	40*	6	35	39	18*	-12	55	16	-7*	-7	204	9	-10	-10	30	36	5*
7	16	36	-15*	7	35	36	32*	-10	19	42	-26*	-6	163	11	-5	-9	110	7	-5
8	15	43	4*	8	60	12	-1*	-8	175	6	-10	-5	299	7	-8	-8	91	7	6
9	117	8	1	9	76	13	17	-6	347	9	-8	-4	207	6	-2	-7	193	6	-10
10	28	43	-6*	10	124	7	1	-4	311	7	4	-3	198	6	2	-6	105	6	1
11	181	6	6	H,K=	12,	7	-2	261	9	-22	-2	90	14	2	-5	268	6	-15	
12	42	28	-5*	-12	0	38	-7*	0	27	41	-26*	-1	62	13	13*	-4	31	40	8*
H,K=	12,	5	-11	8	36	-13*	2	120	8	-6	0	34	44	22*	-3	256	6	-12	
-15	68	15	-5*	-10	0	35	-8*	4	215	9	-3	1	62	22	-1*	-2	18	34	12*
-14	92	8	-6	-9	103	14	10	6	263	6	-2	2	76	9	-10	-1	109	19	-4
-13	34	37	-9*	-8	0	37	-7*	8	247	6	-6	3	114	10	-3	0	48	49	16*
-12	22	36	17*	-7	168	7	-3	10	123	9	-1	4	116	7	-14	1	35	36	-16*
-11	33	35	26*	-6	21	34	19*	12	0	39	-27*	5	169	6	2	2	27	35	4*
-10	72	12	-4	-5	206	6	-3	H,K=	13,	1	6	143	6	-3	3	164	6	4	
-9	121	8	2	-4	0	37	-19*	-17	48	20	41*	7	170	6	-5	4	0	40	-55*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	193	6	3	9	52	42	-6*	-10	11	43	7*	-11	14	38	13*	-7	96	8	-7
6	65	19	13*	H,K=	13,	7		-9	111	7	0	-10	55	15	10*	-6	159	6	-0
7	190	7	0	-11	156	11	-10	-8	0	44	-18*	-9	0	38	-31*	-5	134	6	3
8	50	17	20*	-10	28	38	21*	-7	224	6	-1	-8	212	6	9	-4	138	7	-10
9	151	8	-11	-9	115	11	-19	-6	146	6	-0	-7	65	13	20*	-3	149	6	5
10	0	39	-6*	-8	47	30	37*	-5	284	8	-5	-6	294	7	-2	-2	112	7	-11
11	69	13	-3*	-7	78	10	-13	-4	128	17	-10	-5	35	43	13*	-1	40	46	9*
H,K=	13,	5	-6	0	41	-6*	-3	223	7	2	-4	266	9	-2	0	48	15	9*	
-14	88	12	-2	-5	37	24	31*	-2	35	31	-11*	-3	75	9	10	1	0	58	-22*
-13	108	7	3	-4	44	15	37*	-1	90	15	-1	-2	135	12	-1	2	77	10	9
-12	142	6	-13	-3	99	7	-11	0	15	48	8*	-1	41	24	24*	3	60	13	2*
-11	133	9	8	-2	28	44	7*	1	35	35	-17*	0	25	36	-1*	4	139	6	9
-10	150	6	-9	-1	192	5	-3	2	3	35	-25*	1	35	41	33*	5	93	11	3
-9	108	7	-2	0	0	36	-0*	3	131	6	-4	2	80	9	-1	6	151	6	5
-8	93	9	-9	1	180	5	-5	4	36	30	-15*	3	43	21	12*	7	99	12	-3
-7	20	40	1*	2	40	21	35*	5	176	6	-5	4	174	6	1	8	135	7	-4
-6	57	17	16*	3	145	6	-6	6	89	12	-2	5	0	43	-25*	H,K=	14,	6	
-5	36	47	22*	4	0	49	-7*	7	202	6	-4	6	198	11	7	-11	94	9	-6
-4	63	10	-3	5	80	14	2	8	79	18	-11*	7	34	55	3*	-10	147	7	-2
-3	90	8	-8	6	14	40	11*	9	149	7	-2	8	168	9	4	-9	63	11	9
-2	187	5	-3	H,K=	13,	8		10	58	24	1*	9	40	42	10*	-8	111	7	-5
-1	138	8	-5	-8	115	10	8	11	75	18	13*	10	119	7	10	-7	0	38	-5*
0	196	6	-9	-7	66	15	3*	H,K=	14,	2	11	30	40	14*	-6	30	36	-4*	
1	142	6	-18	-6	155	5	-4	-16	38	40	13*	H,K=	14,	4	-5	39	51	13*	
2	136	6	-11	-5	64	11	-7	-15	81	14	-2	-14	42	26	7*	-4	41	29	-3*
3	115	7	2	-4	152	6	-4	-14	67	27	-8*	-13	159	8	4	-3	22	36	-5*
4	87	8	-5	-3	67	10	3	-13	133	7	-0	-12	48	19	15*	-2	127	8	-9
5	59	15	3*	-2	103	9	-17	-12	129	8	2	-11	190	8	8	-1	85	10	-4
6	28	36	20*	-1	38	51	-0*	-11	162	6	-2	-10	35	47	-3*	0	184	6	9
7	24	37	12*	0	0	36	-22*	-10	128	7	1	-9	191	6	4	1	109	8	5
8	58	35	1*	1	0	37	-4*	-9	141	6	6	-8	7	37	-18*	2	144	6	-5
9	75	11	2	2	67	11	0	-8	79	12	-1	-7	94	12	3	3	74	11	19
10	107	8	4	3	46	22	8*	-7	127	6	3	-6	45	46	8*	4	87	9	1
H,K=	13,	6	H,K=	14,	0	-6	23	36	17*	-5	6	36	3*	5	42	21	17*		
-13	47	17	3*	-16	40	53	-17*	-5	0	41	-25*	-4	0	36	-20*	6	51	16	24*
-12	35	37	16*	-14	166	6	5	-4	51	15	31*	-3	138	6	-1	7	14	49	4*
-11	23	50	9*	-12	217	6	1	-3	147	11	-2	-2	16	35	10*	H,K=	14,	7	
-10	38	27	-27*	-10	228	6	4	-2	122	8	-2	-1	242	6	1	-9	84	12	-10
-9	50	36	-7*	-8	164	7	-5	-1	149	8	-5	0	56	13	7*	-8	18	36	13*
-8	121	6	-12	-6	66	10	13	0	151	6	-7	1	247	7	6	-7	142	9	6
-7	72	10	-18	-4	115	7	-2	1	186	5	2	2	99	7	10	-6	22	41	15*
-6	156	6	-15	-2	178	9	-4	2	175	6	-6	3	183	6	-5	-5	171	8	2
-5	72	9	-8	0	311	7	-3	3	182	6	-13	4	57	19	3*	-4	37	41	18*
-4	181	10	-16	2	297	7	0	4	97	8	-5	5	74	11	-4	-3	162	6	2
-3	56	17	-7*	4	172	8	-5	5	85	10	-7	6	20	38	15*	-2	35	36	24*
-2	118	8	-15	6	48	17	29*	6	31	39	21*	7	52	37	22*	-1	97	9	5
-1	46	15	1*	8	111	7	5	7	0	47	-42*	8	24	42	-6*	0	7	36	6*
0	51	15	18*	10	121	7	-11	8	65	12	-3*	9	107	11	4	1	27	40	10*
1	33	37	9*	12	117	8	-13	9	84	9	-1	10	19	46	-26*	2	25	37	24*
2	50	15	-15*	H,K=	14,	1	10	71	12	-17	H,K=	14,	5	3	97	8	2		
3	54	13	1*	-16	63	14	-2*	11	100	12	-1	-13	44	22	5*	4	22	42	13*
4	140	8	-8	-15	126	7	7	H,K=	14,	3	-12	0	42	-21*	H,K=	14,	8		
5	49	17	-20*	-14	51	18	19*	-15	35	39	6*	-11	34	53	14*	-3	55	14	3*
6	175	6	3	-13	73	12	-3	-14	116	8	-1	-10	44	36	-4*	-2	107	7	-5
7	74	10	0	-12	51	17	14*	-13	27	38	12*	-9	35	45	-28*	-1	65	13	-3*
8	154	6	8	-11	29	49	25*	-12	39	41	-7*	-8	132	6	8	H,K=	15,	0	

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-14	122	9	7	0	30	36	25*	6	50	18	24*	-4	61	11	0	-11	17	49	14*
-12	65	12	12	1	13	36	-16*	7	172	6	3	-2	163	5	2	-10	27	39	-26*
-10	39	42	-20*	2	45	17	-2*	8	51	18	24*	0	216	6	0	-9	7	39	-11*
-8	172	7	5	3	71	14	-3*	H,K=	15,		5	2	207	6	4	-8	135	7	-1
-6	261	7	-8	4	96	9	-3	-12	127	8	7	4	118	6	-0	-7	48	24	9*
-4	326	7	3	5	123	6	4	-11	92	9	3	6	38	26	5*	-6	206	7	4
-2	186	5	-2	6	103	8	-8	-10	140	8	-3	8	49	21	-19*	-5	43	25	-6*
0	33	43	-4*	7	154	6	11	-9	107	9	17	H,K=	16,		1	-4	207	6	10
2	83	15	-4	8	81	12	-6	-8	103	8	-2	-14	46	29	4*	-3	0	44	-30*
4	152	5	8	9	119	9	7	-7	70	18	1*	-13	92	23	24*	-2	157	7	3
6	230	6	3	10	34	39	-20*	-6	0	52	-10*	-12	0	38	-18*	-1	46	30	30*
8	199	6	-3	H,K=	15,		3	-5	0	36	-4*	-11	20	41	11*	0	47	17	8*
10	92	14	-11	-14	106	9	-2	-4	68	13	5*	-10	25	44	18*	1	11	44	-3*
H,K=	15,		1	-13	0	42	-20*	-3	72	17	2*	-9	108	7	6	2	70	20	7*
-15	87	15	8	-12	168	6	-4	-2	113	10	-8	-8	70	10	-2	3	20	41	12*
-14	77	11	7	-11	34	38	-10*	-1	142	6	14	-7	151	6	-9	4	134	6	3
-13	144	7	-1	-10	170	6	6	0	181	7	0	-6	85	9	-4	5	56	19	3*
-12	64	13	-2*	-9	49	17	-1*	1	104	8	-3	-5	190	7	-2	6	152	11	4
-11	174	6	-0	-8	146	10	8	2	154	8	4	-4	105	7	1	7	36	38	4*
-10	74	11	-3	-7	28	37	13*	3	89	10	-4	-3	179	6	-2	H,K=	16,		4
-9	164	6	-1	-6	58	13	5*	4	78	10	10	-2	37	41	-7*	-11	165	6	9
-8	60	16	21*	-5	11	37	-5*	5	36	42	-8*	-1	65	11	-22	-10	29	38	9*
-7	97	11	-6	-4	53	17	8*	6	6	45	-4*	0	44	20	36*	-9	158	6	17
-6	35	41	-1*	-3	0	37	-31*	7	42	25	34*	1	46	24	12*	-8	0	38	-7*
-5	0	37	-5*	-2	167	6	6	H,K=	15,		6	2	33	40	-3*	-7	98	8	4
-4	57	13	-20*	-1	73	12	15	-10	39	47	1*	3	93	12	-10	-6	0	44	-11*
-3	115	8	-7	0	224	6	7	-9	42	49	-13*	4	36	37	-18*	-5	27	37	3*
-2	104	8	8	1	40	30	12*	-8	117	7	6	5	143	6	6	-4	0	40	-12*
-1	221	8	1	2	240	6	10	-7	46	23	-16*	6	79	12	6	-3	119	7	12
0	77	8	2	3	31	38	14*	-6	145	7	-1	7	156	10	-4	-2	41	47	6*
1	246	6	-7	4	160	7	3	-5	70	13	9	8	71	20	-10*	-1	179	6	-1
2	76	9	8	5	28	37	26*	-4	161	7	7	H,K=	16,		2	0	68	16	3*
3	170	5	-2	6	18	37	-0*	-3	64	24	12*	-13	135	11	14	1	196	7	7
4	67	10	7	7	34	54	31*	-2	112	9	-7	-12	113	9	5	2	43	51	-8*
5	53	21	-24*	8	47	49	-22*	-1	60	17	0*	-11	134	8	7	3	152	6	2
6	8	39	-2*	9	0	39	-4*	0	0	37	-24*	-10	110	8	1	4	38	47	10*
7	37	38	8*	H,K=	15,		4	1	26	44	19*	-9	128	8	7	5	82	13	27
8	33	37	-4*	-13	64	47	-5*	2	46	19	-3*	-8	73	14	-6*	6	43	22	41*
9	77	18	-21*	-12	0	40	-23*	3	54	14	4*	-7	86	11	7	H,K=	16,		5
10	51	30	10*	-11	26	40	10*	4	111	9	5	-6	3	41	-19*	-10	27	51	-4*
H,K=	15,		2	-10	33	54	14*	5	74	16	2*	-5	0	37	-17*	-9	75	12	19
-15	100	9	1	-9	92	9	4	H,K=	15,		7	-4	38	26	-4*	-8	100	8	7
-14	77	11	-1	-8	42	24	6*	-6	37	37	32*	-3	96	7	1	-7	82	26	-8*
-13	47	21	-4*	-7	188	8	-12	-5	35	36	24*	-2	117	6	9	-6	131	6	3
-12	10	38	-16*	-6	44	47	10*	-4	15	43	-2*	-1	163	9	8	-5	94	9	-6
-11	60	13	58*	-5	217	6	9	-3	90	14	-5	0	145	7	3	-4	120	7	3
-10	29	43	-18*	-4	55	14	2*	-2	33	36	18*	1	168	6	-2	-3	100	8	6
-9	79	10	-6	-3	179	9	-5	-1	145	10	4	2	122	10	1	-2	94	8	-2
-8	101	8	-4	-2	65	11	16	0	42	21	37*	3	138	7	7	-1	57	18	15*
-7	154	6	6	-1	112	8	13	1	160	8	5	4	71	11	-12	0	31	38	-4*
-6	134	6	6	0	36	37	17*	H,K=	16,		0	5	57	14	-8*	1	37	41	18*
-5	221	6	1	1	31	37	22*	-14	112	8	3	6	0	37	-12*	2	52	20	-2*
-4	127	6	7	2	27	40	-9*	-12	156	10	-7	7	50	14	41*	3	38	42	-0*
-3	147	5	2	3	119	7	4	-10	170	11	-4	8	45	32	8*	4	109	9	-6
-2	77	10	-5	4	0	51	-23*	-8	134	7	6	H,K=	16,		3	H,K=	16,		6
-1	53	23	12*	5	178	7	-1	-6	40	23	-10*	-12	34	39	-4*	-7	10	41	-5*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.(CH5N)2 PAGE19

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	39	27	10*	5	86	9	2	-5	165	6	-4								
-5	50	16	42*	6	109	10	14	-4	67	11	6								
-4	58	14	18*	H,K=	17,		3	-3	119	7	-14								
-3	34	38	-2*	-10	138	9	2	-2	33	43	-3*								
-2	118	10	11	-9	45	20	-3*	-1	59	15	2*								
-1	35	38	-14*	-8	105	11	2	0	49	14	32*								
0	134	7	4	-7	25	49	7*	1	0	50	-11*								
1	46	21	-18*	-6	49	22	9*	2	16	39	3*								
H,K=	17,		0	-5	32	47	21*	3	65	12	-8*								
-12	31	39	-7*	-4	56	20	6*	4	50	16	2*								
-10	42	55	-2*	-3	30	38	10*	H,K=	18,		2								
-8	143	9	7	-2	117	7	-2	-9	85	10	-0								
-6	195	6	-1	-1	51	22	30*	-8	71	11	9								
-4	195	6	1	0	168	6	-2	-7	51	56	-12*								
-2	140	7	2	1	40	47	21*	-6	14	42	-7*								
0	24	43	-30*	2	170	6	5	-5	26	40	20*								
2	58	13	-12*	3	53	15	25*	-4	41	22	16*								
4	153	6	9	4	102	8	1	-3	70	11	-1								
6	167	8	15	5	34	37	10*	-2	84	9	11								
H,K=	17,		1	H,K=	17,		4	-1	89	13	-18								
-12	78	11	2	-9	73	18	-3*	0	106	11	-1								
-11	154	7	6	-8	35	38	6*	1	125	6	6								
-10	86	9	16	-7	140	7	-3	2	89	9	-5								
-9	116	7	-2	-6	26	46	-7*	3	101	8	-6								
-8	44	32	-16*	-5	168	11	4	H,K=	18,		3								
-7	56	14	-12*	-4	2	42	-25*	-7	0	41	-36*								
-6	36	46	21*	-3	131	7	-3	-6	155	6	0								
-5	15	37	11*	-2	60	12	31*	-5	38	40	7*								
-4	34	35	8*	-1	78	10	-1	-4	148	6	9								
-3	79	9	-8	0	36	37	27*	-3	36	37	10*								
-2	64	18	6*	1	24	38	6*	-2	118	14	18								
-1	163	6	-7	2	19	38	-4*	-1	26	40	9*								
0	76	9	8	3	86	10	-4	0	38	32	-6*								
1	180	6	-8	H,K=	17,		5	1	24	42	19*								
2	87	18	4*	-6	47	20	33*	H,K=	18,		4								
3	138	7	3	-5	0	39	-10*	-4	0	54	-7*								
4	55	26	7*	-4	37	42	-5*	-3	61	23	-15*								
5	67	11	7	-3	67	12	22	-2	13	51	-16*								
6	50	23	32*	-2	93	9	-5	H,K=	19,		0								
H,K=	17,		2	-1	102	13	2	-4	153	8	7								
-11	0	38	-2*	0	139	7	14	-2	97	11	7								
-10	28	42	2*	1	94	9	-1	H,K=	19,		1								
-9	65	15	2*	H,K=	18,		0	-5	0	47	-11*								
-8	78	9	7	-10	156	6	14	-4	0	56	-10*								
-7	119	7	-15	-8	101	7	9	-3	73	16	-3*								
-6	121	7	9	-6	50	19	5*	-2	68	16	15*								
-5	150	6	2	-4	0	43	-32*	-1	140	8	10								
-4	124	9	9	-2	131	6	6												
-3	114	7	-8	0	182	6	3												
-2	84	9	6	2	170	12	3												
-1	54	21	-4*	4	102	9	15												
0	0	36	-13*	H,K=	18,		1												
1	34	42	26*	-9	63	15	-1*												
2	50	15	14*	-8	58	19	1*												
3	64	14	1*	-7	127	7	0												
4	83	8	8	-6	85	9	10												

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